Community Air Monitoring Plan
Appendix G

California Statewide Mobile Monitoring Initiative (SMMI) Partner Mobile Laboratory Quality Assurance and Data Management Plan

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July 1, 2025

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The Statewide Mobile Monitoring Initiative is part of California Climate Investments, a statewide initiative that puts billions of Cap-and-Trade dollars to work reducing greenhouse gas emissions, strengthening the economy, and improving public health and the environment — particularly in disadvantaged communities.

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Community Air Monitoring Plan Appendix G.1

California Statewide Mobile Monitoring Initiative (SMMI) Aerodyne Research Quality Assurance and Data Management Plan

Aerodyne Research

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Prepared by Aerodyne Research

In partnership with Aclima

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Contents

1. Key concepts

Data will be collected on board the Aerodyne Mobile Laboratory [1-3] (AML, Figure 1).

Figure 1: The Aerodyne Mobile Laboratory

Table 1: Sample Instrument Manifest for Mobile Measurements by the Aerodyne Mobile Laboratory. Precisions reported at the 1-sigma levels, in parentheses. LODs typically 3 times the precision.

Instrument	Sampling Interval	Species Measured	**RFI Species**	**Reference**
Aerodyne Tunable Infrared Direct Absorption Spectrometers (TILDAS) TILDAS-CS-C_2H_6	1-sec	CH_4 (10 ppb), C_2H_6 (200 ppt)	**CH_4** (10 ppb)	
TILDAS-CS N_2O/CO/H_2O	1-sec	CO (0.1 ppb), N_2O (0.2 ppb), H_2O (10 ppm)	**CO** (0.1 ppb),	
TILDAS-CS-HCHO	1-sec	Formaldehyde (100 ppt)		
TILDAS-FD-EtO	1-sec	Ethylene oxide (75 ppt)		
CAPS-NOx Cavity Attenuated Phase Shift Spectrometers	1-sec	NO_2 (120 ppt), NOx (300 ppt)	**NO_2** (120 ppt), **NOx** (300 ppt)	
LI-COR 6262 CO_2 Non-Dispersive Infrared Carbon Dioxide Analyzer	1-sec	CO_2 (0.5 ppm)	**CO_2** (0.5 ppm)	
2BTech Ozone Monitor Model 205	2-sec	O_3 (2 ppb)	**O_3** (2 ppb)	

Instrument	Sampling Interval	Species Measured	**RFI Species**	**Reference**
Aerodyne Vocus 2R Proton Transfer Reaction Time of Flight Mass Spectrometer (Vocus PTR-ToF)	1-sec	VOCs and HAPs including aromatics (10 – 100 ppt typical precision)	**Benzene, toluene, sum of ethylbenzene and xylenes, acrolein, sulfur containing compounds, Select PAHs, Unspeciated carbonyls,**	
Aerodyne Thermal Desorption Gas Chromatograph Electron Ionization Time of Flight Mass Spectrometer (GC-EI-ToF)	30 min	isomer-speciated aromatics, C3-C12 alkanes, hydrocarbons, halogenated compounds, 1,3-butadiene, and numerous additional HAPs and VCPs, ~35 compounds (1 to 10s ppt typical LOD for a 700 mL preconcentrated sample)	**Benzene, toluene, ethylbenzene, o-xylene, sum of m- and p-xylenes, methyl bromide, 1,3-butadiene**	

Instrument	Sampling Interval	Species Measured	**RFI Species**	**Reference**
Aerodyne Soot Particle Aerosol Mass Spectrometer (SP-AMS)	1-40 sec	Speciated particulate matter mass, sizes < 2.5 microns: Organics (0.3 µg/m^3), Sulfate (0.04 µg/m^3), Nitrate (0.02 µg/m^3), Ammonia (0.02 µg/m^3), Chloride (0.02 µg/m^3), Black Carbon (0.3 µg/m^3), select metals (atomic/elemental) including lead, chromium, arsenic, cadmium, aluminum). Particle sizing by species when in 40 second sample mode.	**Black carbon** (0.3 µg/m^3) **$PM_{2.5}$** **Metals** **Arsenic (elemental)** **Diesel PM, select PAHs**	
TSI Condensation Particle Counter (CPC) Model 3775	1 sec	Particulate matter number count, sizes < 2.5 microns (30 cm^{-3})		
Cooper Xact 625i	5 mins	Elemental Metals, sizes < 2.5 microns: 45 elements total including; Chromium (.002 µg/m^3) Arsenic (.001 µg/m^3) Selenium (.001 µg/m^3) Bromine (.002 µg/m^3) Cadmium (.04 µg/m^3) Antimony (.009 µg/m^3) Mercury (.002 µg/m^3) Lead (.002 µg/m^3)	**Metals** (0.001 – 0.04 µg/m^3 typical precisions) **Arsenic (elemental)** (.001 µg /m^3)	
ARISense small sensor unit with Alphasense Optical Particle Counter Model OPC-N3	10 sec	PM_1, $PM_{2.5}$ (10 µg/m^3), PM_{10} (20 µg/m^3)	**$PM_{2.5}$** (10 µg/m^3), **PM_{10}** (20 µg/m^3)	

Instrument	Sampling Interval	Species Measured	**RFI Species**	**Reference**
Anemometers (RMYoung Ultrasonic Anemometer Model 85004 or Airmar 200WX), GPS compass (Hemisphere Vector V103)	1-sec	Wind Speed and Direction, GPS position, RH and temperature		

A full list of reported parameters is included in an appendix to this document.

List of Acronyms

AML – Aerodyne Mobile Lab
AQS – Air Quality System: EPA format for air quality data
CAPS – Cavity Attenuated Phase Shift Spectrometer
GC-EI-ToF – the online thermal desorption gas chromatograph system (TD-GC) paired with electron ionization time-of-flight mass spectrometer
GPS – Global Positioning System
PI – Principal Investigator
ppb – parts per billion
ppb – parts per trillion
PTR-MS – Proton transfer reaction mass spectrometry
PTR-ToF-MS – Proton transfer reaction time of flight mass spectrometry (used interchangeably with PTR-MS)
QA – Quality Assurance
RAM – Random Access Memory – characterizes a type of data drive that is used for live data transfer
RFI – Request For Information (refers to CARB document)
RH – Relative Humidity
SP-AMS – soot particle aerosol mass spectrometer
TILDAS – Tunable Infrared Laser Direct Absorption Spectrometer
Vocus – Aerodyne brand name of PTR-MS instrument
XRF – Xray fluorescence

1.1 Roles and Responsibilities

The roles and responsibilities for each participant of this project are outlined below:

Tara Yacovitch, Aerodyne PI

- Overall direction of Aerodyne’s sub-contract
- Field measurement planning and logistics including campaign time period, measurement goals, and some logistics

- Project management and reporting to Aclima
- Data Manager, organizing other Data PI's and ensuring complete dataset, formatting and upload
- Data QA of select Aerodyne results, with focus on GPS, wind, select trace gases

Conner Daube, Mobile Lab Lead

- Assist with field measurement logistics including siting, power, staffing
- Aerodyne mobile laboratory vehicle readiness
- Schedule and assist with instrument integration into the Aerodyne mobile lab
- Lead TILDAS trace gas instrument integration in the mobile laboratory

The following instrument leads are defined.
Megan Claflin, GC Lead (GC-EI-ToF-MS instrument)
Ed Fortner, PM Lead (Cooper XRF and AMS instruments)
Anita Avery, PTR Lead (Vocus PTR-ToF-MS instrument)
Tara Yacovitch, TILDAS Lead
Zach Payne, CAPS lead

Each instrument lead will:

- Determine species measured and calibration strategy
- Lead instrument integration into the mobile laboratory
- Assist with logistics of staffing a scientist to run the instrument during field campaign
- Perform data analysis and QA, delivering QA'ed data to data manager
- Serve as Data PI for the instrument dataset
- Contribute to reports as needed

Roles During Active Field Measurements

In addition to the above project roles, during a field measurement campaign, we define the roles below. Each role must be covered. There are only 4-5 seats in the mobile lab; therefore, certain individuals hold multiple roles during the field campaign.

AML Driver

- Has Commercial Driver's License
- Ensures safe driving and compliance with all DOT rules

Field Lead

- Lead scientist in the field at any given time.
- Responsible for daily measurement goals and their alignment with overall project goals.
- Communication with project PI and Aclima on progress or any issues
- Decides when each given site or measurement area has been sufficiently characterized.

Passenger

- Navigates for the AML driver selecting truck-appropriate routes that meet the measurement goals

- Verifies that all instruments and systems are logging and functional
- Takes notes about sites and observations visible through the window

Topic Expert: Each of the following instrument/system types will have an experienced operator.

- Mobile Lab Systems (pumps, computer systems, live GPS and mapping)
- GC-EI-ToF
- Vocus PTR-ToF
- TILDAS
- CAPS-NOx

1.2 PML data levels and Completeness

Aerodyne's data levels are built upon Aclima's defined data levels. The table below lists these levels, pulling examples from Aerodyne's dataset.

Data Level 0a (L0a) is added to describe uncalibrated integrated signal from a sensor and to distinguish it from the raw saved L0 data. For example, a mass spectrometer produces mass spectral files consisting of a matrix of ion intensity per high-resolution channel (L0). During mobile monitoring, this instrument also produces uncalibrated unit mass resolution (UMR) time series for select bins of the mass spectrum (L0a), which is displayed and logged on a central computer in the mobile lab. L0a data is uncalibrated and may be subject to interferences. Nevertheless, L0a data is a useful tool to guide sampling, flag hotspots live, and provide qualitative rapid turnaround results.

Table 2: PML Data Processing Levels. Aerodyne adds level 0a.

Data Level	Name	Definition	Example in Aerodyne Dataset
0	Raw Signal	Original signal produced by the sensor.	raw mass spectral data, archival spectra from laser instruments, logged "NMEA" strings from GPS units.
0a	Raw Integrated Signal	Uncalibrated integrated signal produced by a sensor.	Total ion signal at a given mass-to-charge ratio, with or without placeholder sensitivity applied. Uncalibrated methane concentration from a laser analyzer in ppb.
1	Intermediate geophysical quantities	Derived from Level 0 data using basic physical principles or calibration equations.	Methane concentration in ppb. Calibrated toluene concentration in ppb.

			Concentration of a species not in a calibration tank, derived from a rate constant approach.
2a	Standard geophysical quantities	Estimate using sensor plus associated on-board physical measurements. Includes more advanced data processing steps.	Quantities harmonized by comparing the output of two instruments reporting the same species (e.g. certain aromatic species in Vocus and GC).
2b	Standard geophysical quantities, extended	Similar to Level 2a but using external data sources for artifact correction Not anticipated to be used for SMMI.	n/a
3	Aggregated geospatial quantities	Geospatial data products derived typically from L1, L2a, or L2b data from single pollutant measurements or a combination of multiple pollutants and using standard statistical aggregation approaches of measurements (i.e. mean, median, max, etc)	n/a – led by Aclima
4	Aggregated geospatial quantities combined with modeled spatio-temporal phenomenology	Aggregated geospatial data products derived typically from L1, L2a, or L2b data using advanced statistical modeling methods across space and time. External data sources or contextual information such as meteorological measurements, topographic data, road type, etc may be incorporated.	n/a – led by Aclima

Data Completeness is defined on an instrument-by-instrument basis as the percentage of data collected during the AML's active measurement time. The AML is considered "active" when it is mobile or stationary in a CNC, in transit, or at one if its overnight parking locations ("bases"). The AML is considered "inactive" during planned calibration or maintenance time at the base, during shore-to-generator power swaps or refueling, during spin-up and shut-down time. Routine/automated zero or calibration checks are planned, and these shall not be considered in the completeness calculation. Certain instruments will report 1 second data when mobile and slower data in certain stationary measurements (e.g. we plan to run the SP-AMS in a slower mode that includes sizing in certain stationary settings). This shall not decrease completeness.

If an instrumental problem occurs that impacts data completeness/recovery for more than 30 minutes (excluding planned maintenance and calibrations), the instrument PI will notify the Field Lead as soon as the problem is flagged. The Field Lead will decide whether the daily measurement goals need to be adjusted (e.g. to allow for maintenance, or to re-measure a particular area) or whether measurements shall continue (e.g. if the instrument in question is low-priority for the source in question and/or a fix cannot immediately be executed). Major completeness/recovery problems affecting > 3 hours of data, or that require any adjustment to the CAMPs, will be immediately communicated to the Aerodyne project PI and the Aclima PML lead by the Aerodyne field lead. A joint decision will be made on a mitigation plan. Aclima will notify CARB of any data completeness issues that are likely to impact the success of a CAMP.

1.3 Data management pipeline

Key steps in the PML's data management are summarized in Table 3 below.

Table 3: An overview of the major components of the Aerodyne data management pipeline.

Data management pipeline		
1	**Publish**	[How raw data gets from the instrument to the point of ingestion] Raw instrument data is saved to instrument computer or data logging computer in the Aerodyne Mobile Lab.
2	**Ingest**	[ingestion of data into staging storage] Daily, instrument and data logging computers are synched to a network-accessible drive located in the mobile lab. Periodically, at personnel changes (1-2 weeks during campaign), raw data is carried on an external drive to Aerodyne servers.
3	**Transform**	[transforming data into various forms and formats for use] Data analysis is handled by a team of scientists on their individual computers. Final time-stamped concentration and AQS flag data for each instrument is produced. Then, a data manager will reformat data into "long" format data (time stamp, GPS stamp, and multiple data columns and flag columns). Data manager will run Aclima code to translate data into "short" format for upload to PML data bucket.
4	**Model**	The majority of the modeling is managed by Aclima. Aerodyne will provide scientific review of Aclima data modeling products, and will produce more advanced instrument-specific data figures for reporting purposes as requested by Aclima (e.g. size speciation of a high-priority particulate matter plume; VOC mass spectrum for an unknown odor plume).

5	**Store**	[How data is stored at all stages of the pipeline] Raw data (L0 and L1) is stored in an organized campaign folder on the AML data server; then at Aerodyne; and finally is transmitted to CARB via physical media. Analyzed data products (L1 and L2) will be pushed to an Aerodyne data bucket on google cloud services, and will be backed up on Aerodyne servers.

2. Data ingestion

Data ingestion describes the process by which the unaltered lowest level data from the instruments is delivered to the PML data storage. Data processing is a manual process and is described in "Data Transformation".

Data from all instruments is acquired and stored/logged either on the instrument computer (for mass spectrometers and TILDAS instruments) or on a dedicated logging computer (for meteorological and other 3rd party instruments). This L0 data is the archival data source that will be used for analysis. See "Data Storage" section for further details on the data flow of this archival data. See "Data Transformation" section for details on the process by which acquired data is transformed into calibrated data.

During live acquisition, a *duplicate* copy of select series data is saved as a transient file to one or more shared RAM drives. These transient files are ingested by the main data visualization and mapping computer in the mobile lab. This process is termed "data exchange by file transfer", and abbreviated as "DEFT". This transient data is level L0a or L1, is non-archival and used mainly for live visualization.

3. Data transformation

Data transformation describes how data from instruments, now ingested and stored, is further transformed.

3.1 Data transformation workflows

Each instrument's data will be loaded and quality assured (see Section 6) by an analyst. Varying levels of data transformation are required and are described below for each instrument. A designated data analyst will oversee the production of calibrated mixing ratios for each species in Table 1. They will also be responsible for producing AQS flag data.

An inlet lag correction will be applied to each instrument separately, to correct for the lag time in sample gas reaching the detector through the AML's various inlets. This lag time is determined based on a combination of timed overblows of zero air on the trace-gas inlet line and measured traffic spike data. Short-duration plumes are more accurate than calculated inlet lags, and traffic plumes conveniently contain strong enhancements from nearly all our instruments.

Quality assured GPS position will be associated with the time waves produced by each instrument.

Finally, data and AQS flags will be formatted into a "long" format – where a single time wave is associated with multiple columns of data/ AQS flag pairs. Aclima software will be run to convert "long" format into "short" format.

3.1.1 GC-EI-ToF Processing Workflow

Raw data produced from the online thermal desorption gas chromatograph system (TD-GC) paired with electron ionization time-of-flight mass spectrometric (EI-TOF-MS) detection, hereafter referred to as GC-EI-TOF, will be processed and quality assured by an analyst. The specific data transformation procedures for the GC-EI-TOF are detailed here, while the quality assurance protocols (including calibration procedures) are described in section 6.1.

To transform the data from raw data to concentration data, the following six steps will be completed by the analyst.

1. High resolution mass spectral peak fitting. The first step in the data analysis procedure for the GC-EI-TOF is to conduct the high-resolution peak fitting using mass spectral analysis software (Tofware, Aerodyne Research). This processing will include defining the mass spectral peak shape and width, conducting mass calibration procedures for peak assignment accuracy, and then fitting the data for high resolution peak assignment. The result of this step will transform the data from unit mass resolution (UMR) to high resolution (HR) molecular formulas.
2. Chromatographic peak integrations. After the data has been through HR fitting, the HR processed data will be imported into the chromatographic analysis software (TERN, Aerodyne Research) for peak integrations. The output of this step will be the VOC speciated data for the specified compounds for reporting in counts (cts).
3. Sample volume normalization. The GC metadata (continuous housekeeping data of all GC components including flow controllers, valves, heaters, etc.) will be used to define the exact GC sample start and stop times for each GC cycle. These GC start and stop times, along with the GC sample flow, will be used to calculate the accurate sample volume (cm^3) collected by the GC preconcentration system for each GC sample. The GC-EI-TOF data will be normalized for the sample volume collected by diving the GC signal (cts) by the collected sample volume and then multiplying by the target sample volume. The output of this step will be the VOC speciated data in normalized counts (ncts).

$$GC\ Signal_{ncts,sv} = (GC\ Signal_{cts})\frac{Sample\ Volume_{Target}}{Sample\ Volume_{Collected}}$$

4. Instrument drift correction. The data will then be subjected to a second normalization step, which utilizes the detection of long-lived halocarbons in the atmosphere. These species, which are expected to have no local sources, are used to correct for changes in analyte signal due to instrument drift (e.g., detector wear or environmental changes). For this step, a halocarbon normalization factor ($NF_{halocarbon}$) will be calculated by diving the GC peak area of the halocarbon of choice (e.g., CCl_4) by the average halocarbon peak area for the entire measurement intensive. The GC-EI-TOF data is then corrected by diving the data by the $NF_{halocarbon}$. The output of this step will be the VOC speciated data in normalized counts (ncts), having been corrected for both sample volume and instrument drift.

$$NF_{halocarbon} = \frac{halocarbon_{sig}}{halocarbon_{avg}}$$

$$GC\ Signal_{ncts} = \frac{GC\ Signal_{ncts,sv}}{NF_{halocarbon}}$$

5. Masking zero and calibration periods. During the campaign, the GC-EI-TOF will be regularly taken offline from ambient sampling for instrument zeros and calibrations. These offline periods are expected to occur daily. The data will be masked to include only ambient data. Flags will be provided to mark these periods as having been devoted to instrument zeros and calibrations.
6. Apply analyte sensitivities. Finally, the sensitivities measured from the pre- and post-campaign calibrations (see section 6.1) will be applied to the ambient data to transform the data from normalized counts (ncts) to concentration data (parts per billion, ppb).

3.1.2 Vocus PTR-ToF Processing Workflow

The Vocus proton transfer reactor time of flight mass spectrometer (Vocus PTR-TOF, "Vocus") records mass spectra of bulk VOCs in real time. An analyst will process the data to provide high resolution peak assignments, apply calibration factors for quantitation, and provide quality assurance.

To transform the data from raw data to concentration data, the following steps will be completed by the analyst.

1. High resolution mass spectral peak fitting. The first step in the data analysis procedure for the Vocus is to conduct the high-resolution peak fitting using mass spectral analysis software (Tofware, Aerodyne Research). This processing will include defining the mass spectral peak shape and width, conducting mass calibration procedures for peak assignment accuracy, and then fitting the data for high resolution peak assignment. The result of this step will transform the data from unit mass resolution (UMR) to high resolution (HR) molecular formulas. This step is the same between GC-EI-TOF and Vocus as the same spectral format and processing software (Tofware) are used.
2. Masking zero and calibration periods. During the campaign, the Vocus will be taken offline from ambient sampling for instrument zeros (approx. hourly) and calibrations

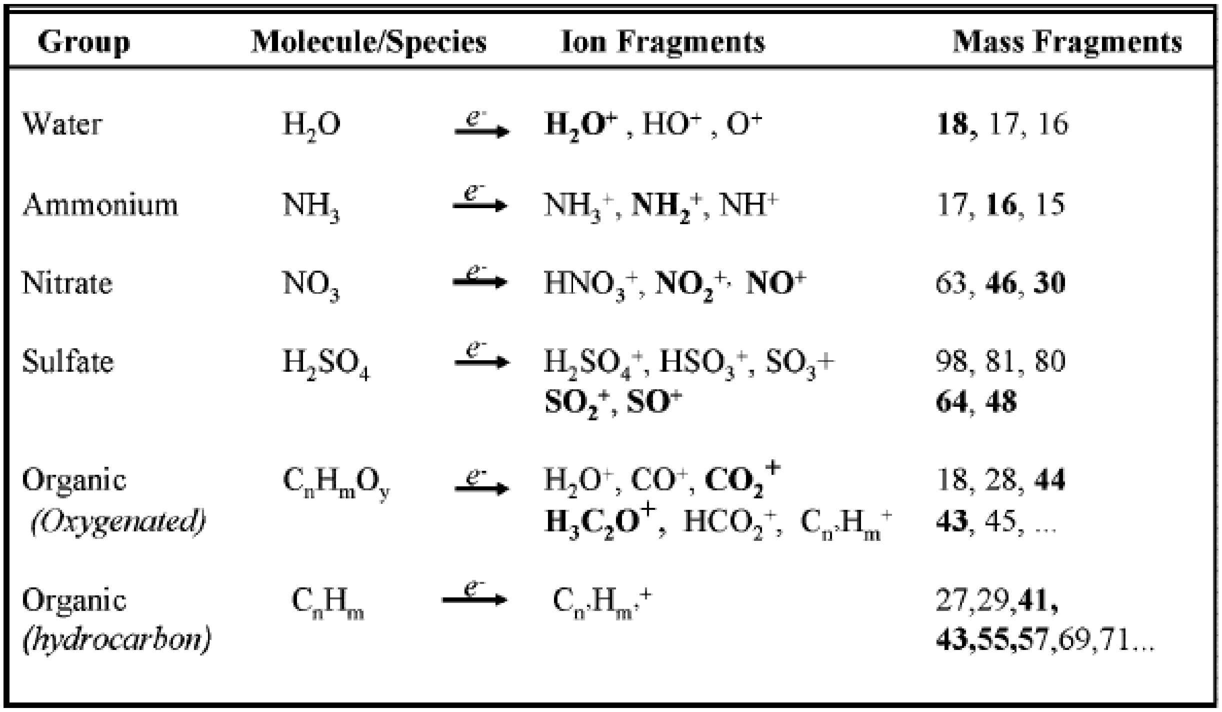
(approx. 6-8x/day). These zeros and calibrations will be flagged for data marking and used in subsequent steps for quantification. The calibrations will be performed with a calibration gas cylinder diluted with zero air. The calibration gas cylinder will contain approximately 15 compounds to provide a sensitivity for those individual compounds.

3. Transmission correction. The Vocus employs a filter to remove low m/z ions from reaching the detector to avoid overloading the detector with reagent ion. The compounds in that calibration tank will be of sufficient m/z range, generally acetonitrile (m/z 42) to D5 siloxane (m/z 371), and sensitivity, that a transmission curve can be created and used to correct the sensitivity of small ions that are not in the tank.
4. Instrument drift correction. Changes in instrument performance will be accounted for by changes in sensitivity to compounds in the calibration tank. Since both changes in absolute sensitivity, (e.g. detector drift) and relative sensitivity due to changes in fragmentation (e.g. reactor conditions), an average of xylene and a-pinene sensitivity changes will be used to apply to other compounds.
5. Apply analyte sensitivities. Sensitivities of each analyte will be applied via the methods described in section 6.1 such that the final data will be reported in concentration data (parts per billion, ppb).

3.1.3 SP-AMS and CPC Processing Workflow

3.1.3.1 SP-AMS

The workflow from raw data to high- resolution quantification of multiple chemical species of particulate matter is lengthy. First, an accurate mass-to-charge (m/z) calibration must be ensured by checking the position of H_2O, N_2, and W ions at mz 18, 28 and 184 respectively. This parameter can and will be set for automatic checking after each data point (run) is completed. Now that the assignment of the entire m/z range is set, certain m/z are assigned to specific chemical families using a fragmentation table. Figure 2 depicts some key species with the common mass fragment attributions.



Group	Molecule/Species		Ion Fragments	Mass Fragments
Water	H_2O	$\xrightarrow{e^-}$	$\mathbf{H_2O^+}$, HO^+ , O^+	**18,** 17, 16
Ammonium	NH_3	$\xrightarrow{e^-}$	NH_3^+, $\mathbf{NH_2^+}$, NH^+	17, **16**, 15
Nitrate	NO_3	$\xrightarrow{e^-}$	HNO_3^+, $\mathbf{NO_2^+}$, $\mathbf{NO^+}$	63, **46**, **30**
Sulfate	H_2SO_4	$\xrightarrow{e^-}$	$H_2SO_4^+$, HSO_3^+, SO_3+ $\mathbf{SO_2^+}$, $\mathbf{SO^+}$	98, 81, 80 **64**, **48**
Organic *(Oxygenated)*	$C_nH_mO_y$	$\xrightarrow{e^-}$	H_2O^+, CO^+, $\mathbf{CO_2^+}$ $\mathbf{H_3C_2O^+}$, HCO_2^+, $C_{n'}H_{m'}^+$	18, 28, **44** **43**, 45, ...
Organic *(hydrocarbon)*	C_nH_m	$\xrightarrow{e^-}$	$C_{n'}H_{m'}^+$	27,29,**41,** **43,55,57**,69,71...

Figure 2: Key aerosol species groups are shown along with their most prevalent fragments by ion chemical formula and m/z

This initial designation of masses into aerosol groups is done automatically in real time while collecting the data. After acquisition, the data is processed by an individual experienced in fitting individual peaks in the mass spectrum and this is where high resolution peak fitting leads to the eventual summation of all high-resolution peaks for a specific species (SO4, NO3, etc.). An example of high-resolution peak fitting is shown in Figure 3. The peaks for the ions C2H3O+ and C3H7+ are clearly fit and this is an example of a technique used at every sampled m/z. This peak fitting leads to improved quantification of species as well as the ability to differentiate between primary organics and oxidized organics and their overall prevalence relative to each other.

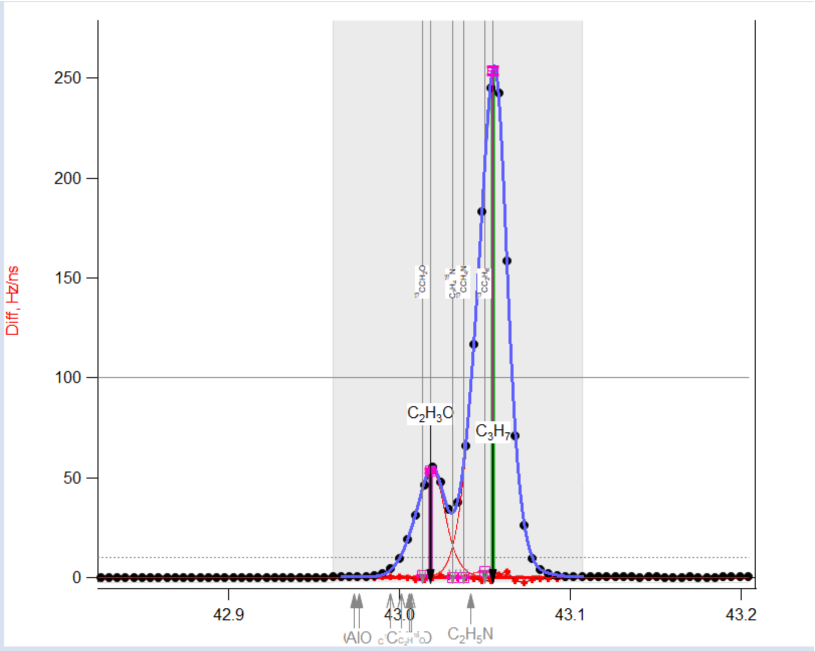


Figure 3: The high resolution fit of the ions $C_2H_3O^+$ and $C_3H_7^+$ at m/z 43 is depicted

Another workflow consideration for the SP-AMS are calibrations. In order to minimize uncertainties in the reported mass concentrations, it is desirable that the fluctuations of the detection efficiency of the AMS are closely monitored and properly corrected throughout the whole campaign. The parameters that capture the AMS detection efficiency are IE_{NO3-}, which is the ionization efficiency (IE) of a reference compound—NO_3^-, and the air beam signal (AB), which is the ion rate (Hz) detected for a major air signal, e.g. N_2^+ in this study. [4, 5] While AB can be monitored continuously during instrument operation, the determination of IE_{NO3-} requires interruption of sampling to perform a calibration experiment (typically 1 – 2 hours). Given this restriction and the expectation (based on previous experience) that IE would not be highly variable, periodic IE_{NO3-} calibrations will be conducted during this study. Because the ratios of IE_{NO3-} to AB remains remarkably constant (r.s.d. < 1%) the continuous AB signal can be used to correct for the variations in the AMS detection efficiencies to a very good approximation.

Two other AMS parameters significantly influence the absolute values of its PM measurements: the collection efficiency (CE) and relative ionization efficiency (RIE). CE is introduced to correct for incomplete detection of nonrefractory particles, NR-PM, by the AMS, e.g., due to irregularly shaped particles that do not completely reach the vaporizer [6, 7]. Although strictly speaking CE should be a function of particle size and shape, at present it is defined as the correction factor for the bulk mass concentrations, i.e., the fraction of the particle mass that is measured by the AMS. A CE value of 0.5 is assigned to sulfate, based on extensive observations from several laboratory and field tests for sulfate aerosols. The same CE value (i.e., 0.5) is applied to particles containing nitrate and ammonium, because they appear to be internally mixed with sulfate particles most of the time.

The CE value for total NR-PM$_1$ organics is estimated based on their size distributions, which often show two modes – a larger accumulation mode of ambient background particles that appears to be internally mixed with SO_4^{2-}, NO_3^- and NH_4^+, and a smaller ultra-fine mode that seems to be mainly emitted from combustion-related sources. A CE value of 0.5 is thus applied to the accumulation mode organics (due to the internal mixing with SO_4^{2-}) and CE for the smaller mode is assumed to be 1.0 because laboratory studies have shown close to 100 % AMS transmission for sooty combustion particles. By studying the size distributions of total organics, as well as individual organics mass fragments averaged over the whole sampling period, we have found that these two modes can be best separated at Dva = 160 nm and that the mass ratio of the smaller (Dva < 160 nm) to the larger mode (Dva > 160 nm) is roughly 2/3. The CE value of the bulk organics is therefore set at 0.7.

Relative ionization efficiency (RIE) is the ratio of the electron impact ionization efficiency of a given species to IE_{NO3}^- on a per unit mass basis. Note that IE_{NO3}^- is the IE of NO_3^- measured based on two major ions, m/z's 30 and 46, instead of all the mass fragments. RIE values representative of individual species have been determined in a range of laboratory measurements and tabulated [8].

The Soot Particle Aerosol Mass Spectrometer (SP-AMS) has the additional capability of measuring refractory black carbon, and this measurement is calibrated by sampling atomized, dried and differential mobility analyzer (DMA) (TSI Model 3081) size selected black carbon (BC) particles into the SP-AMS and a CPC. The ions per picogram of black carbon detected is then compared with the ions per picogram of ammonium nitrate and the RIE of BC is determined by this comparison.[9]

Finally, two other key AMS parameters require calibration. The AMS volumetric sampling flow rate and the particle velocity. The sample flow rate will be determined using a Gilibrator (bubble flowmeter). The particle aerodynamic size reported by the AMS is based on measured particle velocities. The size – velocity calibration is performed using an atomizer with an ammonium nitrate (NH_4NO_3) solution followed by DMA size selection in the range 60 -700 nm.

3.1.3.2 CPC

The commercial Thermo-Systems Incorporated (TSI) condensation particle counter (CPC) is factory calibrated and is periodically returned for refurbishment and recalibration.

3.1.4 Cooper Xact Processing Workflow

The Cooper Xact 625 system is a filter-based measurement. The instrument is factory calibrated, and no further fitting is done to the data. Data blanks are routinely taken by applying a filter to the particulate matter inlet, and these filters are subtracted from the data.

3.1.5 Trace Gas Mixing Ratio Calibration (TILDAS, CAPS and other sensors)

Raw trace gas ratios produced by the trace gas sensors will be reloaded by an analyst and Quality Assured (see Section 6).

Calibration factors determined either pre/post campaign or in-field will be applied to the data. Generally, a single averaged calibration factor will be applied unless there was a marked step-change in instrument response or other issue. Calibrations are only applied if the calibration factor exceeds the uncertainty of the tank.

The resulting calibrated concentration data will output.

3.1.5.1 Trace Gas Calibration Procedures

This section describes a generalized method of performing a dilution calibration. In this procedure, high concentration calibration gas is blended precisely with clean air and delivered to the inlet.

Equipment needed:

1. **Calibration cylinder containing one or more species of interest.** These are commercially available and have typical uncertainties of <1%. Alternate calibration gas sources may be used, including ozone generators.
2. **Clean air to use as a diluent.** For most gas-phase and particulate phase instruments, ultra zero air (UZA) is used (grade containing less than 0.5 ppm of carbon). For certain instruments (e.g. the CAI brand flame ionization detector), a humidity-matched diluent is preferred. In this case, a zero air generator (ZAG) is used. Zero air is generated by passing ambient air through a Aadco ZA30 Catalyst system for destruction of volatile organic hydrocarbons. If performing humid-air calibrations on NOx instrumentation, the zero air will also be passed through Purafill Chemsorbant Media, a potassium permanganate-based scrubber for removal of the oxides of nitrogen (NOx).
3. **Flow measurement device for the calibration gas.** An Alicat mass flow controller capable of delivering up to either 100 or 500 standard cubic centimeters per minute (sccm) will be used to control and measure the delivery of calibration gas.
4. **Flow measurement device for the diluent.** An Alicat mass flow controller capable of delivering up to 20 standard liters per minute (SLPM) will be used to control the delivery of UZA. If using a ZAG, the flow must be manually measured using a flow meter (e.g. DryCal brand) prior to the calibration.

Gas delivery and setup:

Calibration gas is accurately mixed with diluent air before delivery to the inlet. Known quantities of calibration gas and diluent air are combined at a T-shaped fitting a “cal rack” located inside the research vehicle. Electronically-actuated valves allow for easy start and stop of calibration or clean air flow. Alicat mass flow controllers, if used, are at the cal rack. 6 or more feet of 1/2" OD tubing then brings the calibration mixture to the front of the research vehicle, through a port, and to the delivery point within 1 foot of the inlet tip. The use of a long length of wide-bore tubing ensures complete mixing.

The calibration mixture must “overblow” the inlet tip fully. This means that the total flow of calibration mixture must exceed the inlet flow. To ensure an adequate overblow, begin delivering a small amount of diluent air (no calibration gas yet) to the inlet. Observe the live data from a trace gas that is not expected to be present in the diluent gas (e.g. carbon dioxide for UZA) as you gradually increase the flow. The measured trace gas will decrease and then stabilize as the overblow is established. Measure the final flow of diluent gas, either using the Alicat flow controller (if present) or by measuring with a flow meter both the overblow at the inlet tip and the inlet flow during normal sampling. The diluent flow will exceed the known inlet flow.

Perform and work up the calibration:

To begin a calibration, ensure data is being logged and displayed. Note the time, the identity of the calibration cylinder to be used, and the total measured diluent flow. Wait until after any automated instrument backgrounds have completed. Begin delivery of diluent gas. Wait until the instrument-measured concentration has stabilized then collect a minute or so of stable data. Next, begin delivery of the calibration gas by setting the calibration Alicat mass flow controller to the desired flow rate. Note this flow rate in the laboratory book. Typically, it is best to begin at higher cal gas flow rates to help purge the calibration gas line. This first calibration point may take longer than usual to stabilize. Proceed through the calibration, changing the flow of the calibration gas while keeping the diluent gas constant. Make sure to stop the calibration in time for any automated backgrounds. An example calibration time-trace for ethane is shown below.

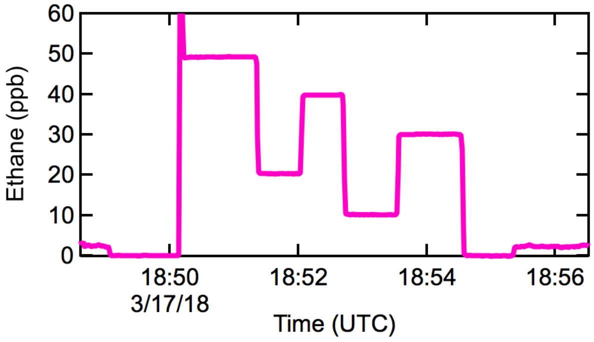


Figure 4: Calibration time trace for ethane

To work up the calibration, determine the concentration of each stable calibration step by averaging the stable periods. Calculate the standard concentration using the known flow rates and known tank concentration. For example, the ethane calibration above used a 1 ppm calibration tank (1000 ppb), calibration flows as noted in the table below (in sccm) and a diluent flow of 8 SLPM (8000 sccm).

std_ethane = 1000*cal_flow/(cal_flow+8000)

Table 4: Calibration data for the example ethane calibration.

cal flow (sccm)	std ethane (ppb)	meas ethane (ppb)
0	0.000	-0.019
500	58.824	49.275

200	24.390	20.305
400	47.619	39.788
100	12.346	10.137
300	36.145	30.099
0	0.000	-0.051
Diluent Flow	8.00 SLPM	

Finally, determine a calibration factor by fitting a plot of measured versus standard concentrations. In this case the calibration factor is 0.838, meaning that the measured concentration must be divided by 0.838 to yield a true concentration. The offset determined during these calibrations is not used, since for most instruments, the zero drifts much more than the range, and is dealt with separately via regular instrument zeroing.

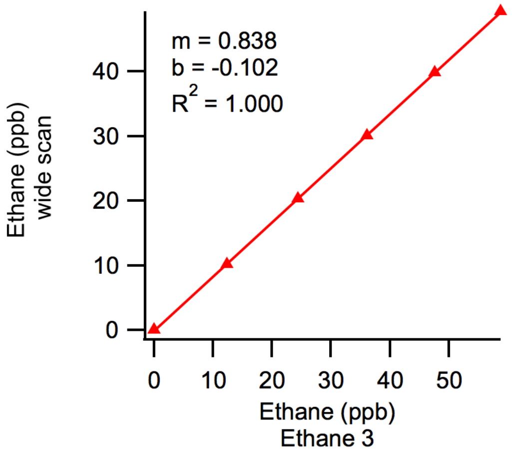


Figure 5: Results of the ethane calibration

As a final step, save a copy of the calibration results (e.g. the graph above) to the project data server under a folder called “calibrations”. If the instrument itself has a log of calibration factors, add the data to this log as well.

Special considerations:

For calibrations of nitrogen oxide (NO), the calibration cylinder regulator and attached tubing must be purged with dry calibration gas before beginning the calibration. This prevents conversion of NO to NO_2 in the presence of water vapor.

When measuring flows with differing instrumentation, ensure that the standard conditions are consistent. For example, the Alicat standard temperature is typically set to 25 C, whereas DryCal flow meters are usually set for a standard temperature of 0 C. Some flow meters do not have temperature sensors, and report just “liters per minute” at the current ambient temperature. Outdoor ambient temperature is measured and logged as part of the meteorological instruments. The temperature inside the vehicle is also logged.

3.1.6 PM2.5 and other loadings

No transformation is required of the PM1, PM2.5 and PM10 values taken directly from an Alphasense OPC-N3 mounted to the AML roof.

3.1.7 GPS and Meteorological Parameter Processing Workflow

3.1.7.1 GPS

No transformation is required of GPS data beyond loading and reformatting into the desired long and short formats.

3.1.7.2 Wind

Raw wind, GPS and heading data are loaded into Igor Pro software, where Aerodyne-written “windMath” software is used to perform the necessary vector math to convert apparent wind to true wind. 2-3 anemometers are used (see Section 6) along with a dedicated GPS compass. For each anemometer, the raw apparent wind is combined with high-quality heading and speed from the GPS compass to yield a true wind corrected for vehicle speed and heading.

4. Data modeling

Aclima will handle the bulk of this project’s data modeling.

Aerodyne will collaborate with Aclima on data visualization related to specific case studies identified during the campaign. Aerodyne will also provide scientific review as requested for any data modeling products produced by Aclima.

4.1 Data modeling workflows

N/A

5. Data storage

Aerodyne has a private data server located at our headquarters in Massachusetts, which is backed up offsite. Aerodyne commits to maintaining this data archive for a minimum of 5 years after the end date of the project. In practice, this archive is maintained indefinitely.

The Aerodyne Mobile Laboratory has a central large volume Synology Network Attached Storage (NAS) drive that is accessible to all instruments on-board and serves as a central spot to back up instrument data. Instrument data is backed up to the NAS daily. At the end of each field intensive, the project folder on the NAS is copied over to Aerodyne's "silo" server. Individual instrument sub-folders are also duplicated to external drives for use during data analysis/transformation and QA.

Level 0 data to be stored includes raw mass spectral files from the Vocus-PTR-ToF, the GC-EI-ToF and the SP-AMS (e.g. .h5 format files), and raw spectral data from TILDAS instruments (.SPE and .SPB files).

6. Data review and quality assurance

Data Quality Assurance will be done instrument-by-instrument by a designated instrument PI. Each PI will be responsible for filling out a section of the QA/QC document that will accompany the dataset delivered to Aclima.

The template QA/QC section for each instrument is as follows:

- Instrument Name
- Data PI name and contact email
- Other contributing scientist names for the purpose of authorship/acknowledgement in publications
- Method description including instrument model
- [Table]: Parameter, full name, description, units, LOD at specified timescale
- [Figure]: Time series for 1 or more parameters covering entire campaign
- Data Analysis and Quality Assurance Description: Include calibration results, identification of data problems, caveats for users. Other figures as needed.
- Sample data line (short format) including header

Each PI will also be responsible for creating the status_indicator code accompanying each dataset, and associated qualifier_code. Descriptions of these parameters, and qualifier codes are included below.

status_indicator	INTEGER	An integer value that represents a boolean (either 0 → false or 1 → true). A value of 1 indicates that this measurement has been flagged,

		meaning there is a relevant annotation (in qualifier_code) that contextualizes data quality or conditions.
qualifier_code	STRING	This field is a blob of comma-separated qualifier codes that documents the reason that data was excluded or flags any notable conditions annotated via the qualifier codes. Routine instrument check data such as calibrations and zeroes will be flagged, and data will be blank. Other invalidated ambient data such as self-sampling of the mobile laboratory's own exhaust will be reported.

Example qualifier codes that may be relevant to Aerodyne datasets are listed below. Additional qualifiers are available at the EPA sites https://www.epa.gov/aqs/aqs-code-list and https://aqs.epa.gov/aqsweb/documents/codetables/qualifiers.html.

Table 5: Select qualifier_codes that may be relevant to Aerodyne Data

Qualifier Code	Qualifier Description	Qualifier Type	Qualifier Type Code
1	Deviation from a CFR/Critical Criteria Requirement.	Quality Assurance Qualifier	QA
2	Operational Deviation.	Quality Assurance Qualifier	QA
3	Field Issue.	Quality Assurance Qualifier	QA
4	Lab Issue.	Quality Assurance Qualifier	QA
5	Outlier.	Quality Assurance Qualifier	QA
6	QAPP Issue.	Quality Assurance Qualifier	QA
7	Below Lowest Calibration Level.	Quality Assurance Qualifier	QA
8	QA/QC Unknown.	Quality Assurance Qualifier	QA
9	Negative value detected - zero reported.	Quality Assurance Qualifier	QA
MB	Method Blank (Analytical).	Null Data Qualifier	NULL
MD	Value less than MDL.	Quality Assurance Qualifier	QA
MS	Value reported is 1/2 MDL substituted.	Quality Assurance Qualifier	QA
SS	Value substituted from secondary monitor.	Quality Assurance Qualifier	QA
AT	Calibration.	Null Data Qualifier	NULL
AS	Poor Quality Assurance Results.	Null Data Qualifier	NULL
AL	Voided by Operator.	Null Data Qualifier	NULL
BA	Maintenance/Routine Repairs.	Null Data Qualifier	NULL
BC	Multi-point Calibration.	Null Data Qualifier	NULL
BD	Auto Calibration.	Null Data Qualifier	NULL
BJ	Operator Error.	Null Data Qualifier	NULL

BK	Site computer/data logger down.	Null Data Qualifier	NULL
AY	Q C Control Points (zero/span).	Null Data Qualifier	NULL

A summary of the calibration and zero frequency for each instrument is listed in the Table below.

Table 6. Summary of calibration schedules performed for each instrument. Further details can be found in sections 6.1 – 6.8.

Instrument	Calibration Schedule
Aerodyne Tunable Infrared Direct Absorption Spectrometers (TILDAS) TILDAS-CS-C_2H_6	Automated backgrounds and zeroes performed every 15 minutes. Manual calibrations performed on designated calibration days, at least 3 times during 6.8 week campaign.
TILDAS-CS N_2O/CO/H_2O	Automated backgrounds and zeroes performed every 15 minutes. Manual calibrations performed on designated calibration days, at least 3 times during 6.8 week campaign.
TILDAS-CS-HCHO	Automated backgrounds and zeroes performed every 15 minutes. Calibration planned once at end of campaign using collaborator tank.
TILDAS-FD-EtO	Automated backgrounds and zeroes performed every 2 minutes when far from a source; every 15 minutes when performing fenceline measurements of a source. Manual calibrations performed on designated calibration days, at least 3 times during 6.8 week campaign.
CAPS-NO_2 and CAPS-NOx Cavity Attenuated Phase Shift Spectrometers	Automated zeroes every 1 hour minutes. Calibrations performed once prior to the campaign and once after.
LI-COR 6262 CO_2 Non-Dispersive Infrared Carbon Dioxide Analyzer	Automated zeroes performed every 15 minutes. Manual calibrations performed on designated calibration days, at least 3 times during 6.8 week campaign.
2BTech Ozone Monitor	Automated backgrounds and zeroes performed every 15 minutes. Calibration performed once prior to the campaign.
Vocus 2R Proton Transfer Reaction Time of Flight Mass Spectrometer (Vocus PTR-ToF)	During campaign: automated zeroes performed every 90 minutes. Automated single point calibrations performed every 3 hours with leading and trailing instrument zeros. Pre- and post- campaign 3 point calibration curve with leading and trailing instrument zeros.
Aerodyne Thermal Desorption Gas Chromatograph Electron Ionization Time of Flight Mass Spectrometer (GC-EI-ToF)	During campaign: Daily, duplicate, single point calibrations with leading and trailing instrument zeros. Pre-, mid-, post- campaign: 5-point calibration curve with triplicate data with leading and trailing instrument zeros.

Aerodyne Soot Particle Aerosol Mass Spectrometer (SP-AMS)	Manual calibrations performed on designated calibration days, at least 3 times during 6.8 week campaign.
TSI Condensation Particle Counter (CPC)	Instrument periodically factory certified.
Cooper Xact 625i	Instrument factory certified prior to campaign.
ARISense small sensor unit with Alphasense Optical Particle Counter	Instrument periodically factory certified.
RMYoung or Airmar Anemometers, GPS compass	No calibration. Duplicate continuous wind measurements used to verify wind direction and magnitude measurement.

6.1 GC-EI-ToF

6.1.1 In-Field GC-EI-ToF

During the campaign, a scientist will be routinely monitoring the GC-EI-TOF components to gauge instrument health and operation. For the EI-TOF-MS, these routine checks will include monitoring the pressure, temperature, and emission current of the ion source and conducting routine checks on the detector strength by measuring the single ion strength (SIS) and then modifying the detector (multi-channel plate) voltage to keep this SIS value stable. The TD-GC will be monitored for flow stability of the carrier, zero, and calibration gases used. This will include daily calibration flow checks. The TD-GC will also be monitored for heater function and control for all heaters, including those used for the columns, thermal desorption traps, and heated transfer areas. The collected sample volume of the TD-GC will be monitored so that any changes due to flow path restrictions or inlet pressure drops can be addressed promptly.

During the field campaign the GC-EI-TOF will undergo regular maintenance by a scientist every ~ 250 GC cycles. With a typical sampling schedule (30 min GC cycle, operating continuously) this equates to maintenance being done every ~ 5 days. This regular maintenance will include installing new adsorbent sample tubes into the first stage of the TD system and adding a new aliquot of conditioned $NaSO_3$ to the oxidant trap, which is used to prevent sampling artifacts (from ambient pollutants such as O_3) ahead of the preconcentration steps.

During the campaign, the GC-EI-TOF will be regularly taken offline from ambient sampling for instrument zeros and calibrations. These zero and calibration periods will occur daily during non-mobile activity. The daily calibration checks will be single point (single concentration) performed in duplicate, with leading and trailing zeros to check instrument residuals.

Before and after the campaign, 5-point calibration curves with triplicates per concentration step will be acquired to confirm the sensitivity and linearity of the system. These calibration curves will have leading and trailing instrument zeros to quantify instrument residuals. Depending on the schedule of the measurement campaign, multi-point calibrations may also be conducted in the middle of the campaign during non-mobile activity.

6.1.2 Post-Analysis of GC-EI-TOF data

Details of the data analysis/transformation process for the GC-EI-TOF data is described in section 3.1.1. Aside from these procedures, and the quality assurance steps there-in, the following data quality metrics will be applied to define any data to be excluded from the reported, final data.

1. As described in section 3.1.1, data acquired during daily instrument zero and calibrations checks will be masked from the reported (ambient) data. These data period will be appropriately flagged as the instrument being offline from ambient measurements for quality assurance protocols (zero and calibrations).
2. During the chromatographic integrations, if there was no peak integrated in the analysis software (TERN, Aerodyne Research) due to low signal, or no signal, above the baseline, then no data (NaN) will be reported. This data will be given a flag for no data reported due to no data fit.
3. Finally, GC-EI-TOF data that does have sufficient signal to be integrated but is below a pre-defined limit of detection (LOD) for that analyte will be flagged as below-LOD and will be removed from the reported/final ambient data.

It should also be noted that while the GC-EI-TOF data will be on its own time basis, the GC sample start and stop times will be provided with the final data for clarity. If requested, the GC-EI-TOF data can also be reported on a campaign time basis (e.g., 1 min) to ease the comparison with the other reported measurements.

6.2 Vocus PTR-ToF

6.2.1 In-Field PTR-ToF Checks

During field data collection, the following checks are performed approximately weekly, up do daily as needed. Note that a new single point calibration described in section 3 is performed immediately after any change is made.

1. Inlet flow check. The inlet can be clogged by atmospheric aerosols blocking the capillary. If the flow is more than 20% clogged, the capillary is replaced.
2. Detector response. The single ion signal (SIS) is measured and it is different by more than 10%, the multichannel plate (MCP) will be increased to keep the SIS consistent.

3. Zero and cal gas flow. The zero and cal gas MFCs are calibrated with an independent method such as a gilibrator to enable a correct quantification of the concentration of cal gas being delivered during calibration.
4. Basic instrument operation checks. During calibration, the raw data is checked for basic sensitivity and fragmentation.

For daily operation during the campaign, the Vocus will sample an instrument zero for 60s every 90 minutes, and will sample a sequence of zero, calibration gas, and zero for 60s each, every 3 hours.

Before and after the campaign, 3 point calibration curves with corresponding zeros will be performed. This calibration can be repeated during the campaign in the case of a hardware failure that results in a re-tuning of the instrument.

6.2.2 Post-Analysis PTR-ToF data

The Vocus provides fast detection of a variety of VOCs with proton transfer ionization (+H+). However, it provides only molecular formula without any structural or isomer information, and many compounds (M) are detected as fragments instead of or in addition to M+H+. The following are techniques for converting the signal described in section 3 in counts to ppb.

6.2.2.1 Directly Calibrated Species

Regular calibrations are carried out using a tank of known compounds at precise and known concentrations. The tank has approximately 15 compounds in it, with a range of molecular weights and compound classes. As a result of delivering this gas at a known concentration to the Vocus, the response of the instrument to that compound can be obtained. This data is then used for transmission and sensitivity calibration as described in section 3. For these compounds, the concentration for that ion (e.g. C3H7O+) is reported using the sensitivity to the calibrated isomer like acetone, with discussion of the potential contribution of other isomers like propanal.
Other direct calibrations of individual compounds that are not in the in-field tank can be carried out before and after measurements. The relative sensitivity during field measurements can be accounted for via the change in the in-field tank.

6.2.2.2 Species Concentrations via Rate Constants

Many species are detected without having a direct calibrant accessible. For these compounds, the linear relationship between sensitivity and the proton transfer rate coefficient is used to estimate the sensitivity. Libraries of PTR reaction coefficients are used,[10] along with an assumption of a single compound or combination of isomers to determine a rate coefficient for the ion detected. The additional uncertainties associated with these assumptions are reported.

6.3 SP-AMS and CPC

The SP-AMS Quality Assurance will consist of examining the data which has already gone through the data transformation process described in Section 3.1.3 above and perform further checks to ensure data reported is meaningful. The data streams will be edited to exclude time periods when calibrations were occurring as well as time periods when filters (zero checks) were being conducted. Filters will be conducted daily with a particle filter at the inlet to ensure there are leaks in the line. The CPC which is measuring on this line will drop to zero counts with the filter at the inlet as long as there are no leaks on the line. Time periods with reduced flow due to a clogging inlet will also be removed from the data.

6.3.1 Particulate Matter Sizing via SP-AMS

Particulate matter sizing will be conducted intermittently with the SP-AMS. The particle sizing when mobile by default will be conducted every 5 minutes for a time period of 40 seconds. When stationary, it is not necessary to run in Fast Mass Spec mode, and this enables more time to sample particle sizing. The particle sizing will be conducted using parameters determined during the velocity-sizing calibration described in section 3.1.3. Particle sizing data is not reported via the standard parameters, but figures showing the size distribution for a given measured plume of interest (e.g. exhaust from a welding shop) will be generated and provided to Aclima for data story purposes. The SP-AMS will be operated with a PM2.5 lens allowing for enhanced detection of larger particles such as metals relative to the standard PM1 lens.

6.4 Cooper Xact

The Cooper Environmental Services (CES) XACT 625 monitor is used to measure particulate matter metals. This is a filter-based X-ray fluorescence method.

This instrument reports several additional parameters beyond the metals and their uncertainties, including alarm status, filter tape status, filament voltage, sample type, measured flow at ambient and at standard temperatures, enclosure and other temperatures, etc. These parameters will be used to QA the reported data, and flag or exclude relevant data points.

As described above for the AMS and CPC instruments, manual blanks are taken routinely during the campaign to ensure that there are no leaks in the sampling line. A blank is done by affixing a filter to the instrument’s inlet. Blanks will be removed from the reported data and indicated by an appropriate qualifier code.

Transmission of large particles through a sampling line necessarily will involve some line losses. These losses are expected to be minimal when the sampling line includes a 2.5 µm cutoff, but may be significant when sampling larger particle sizes up to 10 µm. Line losses will be characterized, and impacted data indicated by a qualifier code and reported in the QA document accompanying the data. We plan for the ability to report either 10 µm or 2.5 µm cutoff data from this instrument, but not both. 10 µm data is more relevant for the measurement of particulate matter metals in lofted dust, whereas 2.5 µm data is more relevant for the measurement of vehicular or other small-particle sources.

6.5 Trace Gas Mixing Ratios

6.5.1 TILDAS: In-Field Instrument Routine Checks.

A scientist will check in on the TILDAS on a daily basis while in the field. These checks will consist of a routine instrument check (aka "Status Check"). More detailed description of the status check procedures are available in the TILDAS Hardware Manual.

Table 6: Status check steps, acceptance criteria and corrective action for the min-TILDAS HCN monitor

Confirm Stream Mode is active	Stream Mode Active	Activate Stream Mode and frequency lock.
Check the laser temperature and laser current	Within 5% of expected value shown in notes.txt file	Load old .con file or manually adjust laser settings
Check the light level	Within 20 % of value on first day of field campaign	Assess noise performance. If warranted, perform laser alignment
Load and inspect your data	Data is complete. Mixing ratios are not negative or unphysically high. Mixing ratios are not correlated to system conditions. Noise meets specification	Negative mixing ratios may indicate insufficient or empty UZA tank – change tank. Assess light level and instrument alignment. Inspect and adjust spectral fit.
Check the gas pressure in the sample cell	Within 0.1 Torr of setpoint	Check pressure controller. Check inlet/filter for clogs. Check filter cleanliness. Change filter and clear inlet if required, following manual procedures.
Check the sample flow rate	Within 0.1 SLPM of setpoint	Check sample pressure. Check inlet/filter for clogs. Re-set flow rate using flow meter and ensure complete overblow during UZA autobackgrounds.
Check the temperature of the sample cell	Similar to ambient temperature	Check mobile lab climate control.

Check the quality of the spectral fit	Blue fit line matches green measured data. Large tuning rate problems may change effective calibration factor.	Load old con file. Check that frequency lock is active. Adjust tuning rate following manual procedures. Adjust fit parameters.
Check the particle filter	Not clogged.	Change filter, following shutdown procedures to safely vent cell. Filter changes typically done weekly.
Check the liquid level of the Oasis chiller	Liquid level is visible. Oasis does not read “tank level low”	Check for coolant leaks. Add Koolance chiller fluid to fill-line.
Confirm that proper Toggle controls are active	WD, ASS, FLK4, PL, ABG are active (purple). RS *may* be active.	Click button to toggle.
Confirm all required schedules and scripts are activated	Schedules unlikely, but possible. To be determined during instrument install.	Enable checkboxes.

The instrument noise is assessed by way of an Allan-Werle variance plot [11]. This can be generated on the instrument computer. Data streamed into the main data visualization computer can also be used for instrument noise performance checks.

6.5.2 TILDAS Post-Acquisition Quality Assurance

After acquisition, the saved L1 TILDAS files containing mixing ratios (.STR files) and instrument conditions (.STC files) are re-loaded by a data analyst in Wavemetrics Igor Pro.

The raw data collected using the protocols described above will be processed to remove and flag (via qualifier code) any manually triggered zeros and calibration checks. Data will be time-corrected to remove the inlet lag (the time taken for ambient air at the inlet tip to reach the monitor), typically less than 3 seconds. Saved instrument conditions (.STC files) will be used to further filter out invalid data. Parameters typically used for QA include peak position, quality of the spectral fit, and sample pressure.

The above inspection will reveal whether any post-analysis of the archival spectral data (L0 data, .SPE and .SPB file pairs) is warranted. Archival spectral data is analyzed in the same software used by the instruments, TDLWintel (see TDLWintel Software Manual, available at support.aerodyne.com). This analysis case is unlikely. Some examples when the archival data is used include:

- UZA tank ran out and data was acquired with an ambient air background.
  Solution: Refit the raw un-backgrounded files to recover the ambient measured data
- High-concentration plume of VOCs causes unexpected interference in the spectrum.
  Solution: Refit the collected spectral files, altering the fit to either exclude the interfering spectral region, or fit additional absorption lines.

Calibration factors for TILDAS species will be calculated from the multi-point calibrations described in Section 3. Factors will be applied if the correction exceeds the stated uncertainty of the calibration tank.

6.5.3 Other Trace Gas Species: In-Field Instrument Checks

A Licor-6262 CO_2 monitor and a 2BTech 502 Ozone monitor report CO_2 and Ozone, respectively. An Aerodyne CAPS-NOx instrument reports total NOx. The functionality of these trace gas sensors is checked routinely via zero and span checks while in the field.

The Aerodyne CAPS NO_x-NO_2 monitor used Cavity Attenuated Phase-shift Spectroscopy (CAPS) technique to measure optical loss in a cavity to determine absolute mixing ratios of NO_2. Baseline (NO_2 free) optical loss is measured frequently (5-15 mins) as a proxy for cavity pathlength and mirror reflectivity. High values for baseline loss indicate mirror contamination. Mirrors can become contaminated due to acid gas attack, high relative humidity, or particle deposition. If values for baseline loss exceed 800 Mm^{-1}, mirrors should be removed and cleaned using lens wipes and HPLC grade methanol.

The span of the CAPS NO_x-NO_2 monitor is tied to the absorption cross-section of NO_2 and minor instrument effects. To this end, the monitor requires infrequent calibrations as the span value typical remains within 5% of its original setting (within the accuracy of the instrument). The monitor is calibrated both before and after the campaign using EPA certified NO_2 in air and validated against ozone titration into verified by an EPA certified ozone photometer.

The Aerodyne CAPS-NOx-NO_2 instrument relies on quantitative conversion of NO into NO_2 and subsequent detection of total NO_2 via Cavity-Attenuated Phase-Shift (CAPS). The functionality of the ozone generator must be verified routinely. This is done through calibration with nitric oxide or through measurements by an ozone monitor (e.g., 2Btech model 707).

The Ozone monitor has a known interference to high concentration VOCs. This interference is mitigated by an internal scrubber.

6.5.4 Other Trace Gas Species: Post-Analysis Quality Assurance

Data is reloaded by an analyst and inspected for glitches or other spurious data points.

Routine instrument zeroes are subtracted from the dataset. Calibration factors are applied. The concentrations of ozone and NOx are plotted together to verify that the expected anti-correlation is present, whereby NOx plumes will titrate away ambient ozone.

CAPS baseline measurements are affected by changes in temperature and pressure. As such, changes in the true baseline can occur during NO_x-NO_2 measurements that are not corrected for until the next baseline. To account for this, linear baseline interpolation is performed on the full data set and corrected values NO_2, NO_x, and NO are provided alongside the raw data.

6.6 PM2.5 and PM10

The Alphasense OPC-N3, in addition to reporting integrated values for PM1, PM2.5 and PM10 in $\mu g/m^3$, also reports particle count by size bin. These size matrices will be re-integrated and processed, and compared to the unit's own output.

6.7 GPS and Meteorological Parameters

The convention for wind is to plot the incident direction, in degrees clockwise from true north. Wind components in the east and north directions may be included for convenience. This convention means that a wind direction of 45 degrees indicates wind *from* the NE (going *to* the SW).

At least 2 replicate wind measurements will be collected on the mobile lab (3 wind devices are shown in Figure 6). The 2D RMYoung ultrasonic anemometer (Model 85004) is the primary reported wind data in the data. Legal limits to the AML height prevent lofting this anemometer any further up, and so **wind data while in motion are impacted by the body of the truck and are often biased**. A dedicated GPS compass (with two internal GPS sensors) is used for accurate GPS data and, more importantly, truck heading. This heading is used in the data transformation of apparent wind into true wind, corrected for vehicle speed and heading. An Airmar 200WX provides redundant GPS and wind data.

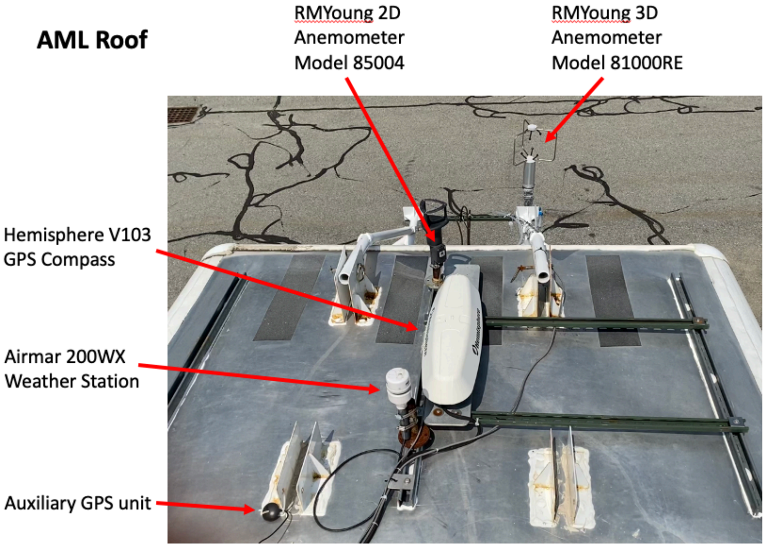


Figure 6: AML Roofline circe 2021

QA is done by comparing wind sensors to each other. The Airmar also outputs true wind speed using its own internal GPS, though we find the heading from this unit can be spotty. The calculated true wind from the Airmar and GPS compass can thus be compared to the reported true wind speed and direction calculated and reported by the device itself. Aerodyne's windMath software includes options for sensor calibration and direction offset correction if the anemometer is slightly rotated off-axis.

Table 7: Meteorological parameter outputs and descriptions

Name	**Description**
wind_E_metersPerSecond	Incident wind component from the east in meters per second. Measured with the RMYoung 2D ultrasonic anemometer (model 85004) and corrected for truck heading and speed.
wind_N_metersPerSecond	Incident wind component from the north, in meters per second. Measured with the RMYoung 2D ultrasonic anemometer (model 85004) and corrected for truck heading and speed.
wind_dir_degrees	Incident wind direction, in degrees clockwise from true north. Measured with the RMYoung 2D ultrasonic anemometer (model 85004) and corrected for truck heading and speed.
wind_speed_MetersPerSecond	Wind speed, in meters per second. Measured with the RMYoung 2D ultrasonic anemometer (model 85004) and corrected for truck heading and speed.
Temperature_C	Degrees C. Outdoor temperature
Pressure Bar	Bar. Outdoor pressure

6.8 Operator Notes and Other Metadata

The nature of the AML measurements – vehicle operated by multiple scientists with research-grade instruments – means that there is a wealth of operator-logged notes. Two types of notes are produced in-field: daily "Captains Logs" which describe daily sampling goals, weather and personnel, status of instruments, and contain a time-stamped log of manual operator notes. This can include descriptions of the sources viewed from the passenger window, particular smells, and preliminary attribution or characterization of plumes.

Second, a start-stop tagged set of notes is kept. These start-stop notes identify manual calibration periods; sections of data in need of QA; and different types of manually-identified plumes (e.g. traffic plumes; natural gas leaks; VOC plumes; etc). Time periods when the generator from the AML may have been sampled are noted by the passenger of the AML in-field and reported along with this start-stop list. Since traffic data is of high interest to this campaign, we will not undertake additional automated filtering of traffic data. However, filters based on CO and NOx concentration enhancements have been used in the past, and those algorithms are available upon request.

The combination of these two types of operator notes will be archived with the L0 data, and delivered to CARB with that L0 dataset. They will be used by Aerodyne as part of data QA and to create qualifier codes.

6.9 Data revisions

It is most efficient to perform data analysis in batches, and so a long 6.8-week measurement campaign will likely be split in 2 or 3 batches. These splits are likely to happen mid-month, and so we expect data revisions when a month's data file is updated to include additional data.

Though all efforts will be made to produce high-quality calibrated results following the data cadence described in this document, occasional revisions may occur. These are often revision of a calibration factor based on intercomparisons with other datasets.

Revisions will include the revision number in the filename (e.g. "r2"), and will be documented in the README file accompanying the data in the data buckets. If the change is substantial (e.g. a calibration factor change, not just data addition), the QA .pdf document will be updated as well.

7. Data transfer

Level 0 data collected by Aerodyne will be delivered to CARB at the end of each field intensive via a mailed or hand-delivered physical storage (e.g. USB key). This raw data will consist of a copy of the project folder maintained on the Aerodyne Mobile Lab's central data server NAS. This Level 0 data includes raw mass spectral files from the Vocus-PTR-ToF, the SP-AMS and the GC-EI-ToF (e.g. .h5 files) and archival spectra collected by the TILDAS instruments (e.g. .SPE, .SPB). This Level 0 data is un-calibrated and not QA/QC'ed.

Higher levels of data (mixing ratios, calibrated results, etc.) will be transferred to Aclima, and the transfer to CARB described in Aclima's Data Transfer Section.

7.1 Data Schema

The Aerodyne Mobile Lab analyzed data will follow the Aclima data schema defined previously. Where possible, standard AQS parameters and method codes are reported. However, most of the instruments have no defined AQS method, and a few reported species have no defined AQS parameter. A new AQS parameter and/or method code will be assigned to those specific data streams for this project, as dictated by Aclima and/or CARB. The list of parameter names are provided as a supplementary spreadsheet.

Table 8: Data schema for the Aerodyne Mobile Lab

Field Name	Field Type	Field Description
timestamp	STRING	The ISO 8601 encoded UTC timestamp at which the measurement was taken with timezone information. The format string is *YYYY-MM-DDTHH:mm:SSZ* (e.g. *2024-09-03T14:46:39Z*)
parameter	STRING	The measurement described by the row, typically pollutant (e.g. ch4, co). For each parameter value, a separate lookup table links this field to AQS parameter codes (1:1 relationship) and a longer text description.
method	STRING	A method identifier for the sensor used to collect the measurement. Most Aerodyne measurements do not have defined method codes, and so the AQS method codes will be extended for this project as needed. For each method value, a separate lookup table links this field to the relevant AQS method code (1:1 relationship) and a longer text description.
duration	INTEGER	Sample duration for the associated measurement. This is relevant in particular for certain methods that require sampling times longer than 1 second or may have variable sampling times over the course of the data collection period. In these cases, the timestamp field represents the start of the sampling period.
value	FLOAT	The measurement value for the measurement parameter at the timestamp in the location.
unit	STRING	The unit of measurement that value represents.

latitude	FLOAT	The latitude at which the measurement was taken. This is used in conjunction with longitude to completely describe the corrected position of the measurement.
longitude	FLOAT	The longitude at which the measurement was taken. This is used in conjunction with latitude to completely describe the corrected position of the measurement
status_indicator	INTEGER	An integer value that represents a boolean (either 0 → false or 1 → true). A value of 1 indicates that this measurement has been flagged, meaning there is a relevant annotation (in qualifier_code) that contextualizes data quality or conditions.
qualifier_code	STRING	This field is a blob of comma-separated qualifier codes that documents the reason that data was excluded or flags any notable conditions annotated via AQS codes. Data is reported for all times that instruments are on during the mobile intensive measurement period, including when the vehicle is stationary. Routine instrument check data such as calibrations and zeroes will be AQS flagged, and data will be blank. Other invalidated ambient data such as self-sampling of the mobile laboratory's own exhaust *will* be reported.
vehicle_id	STRING	A string that uniquely identifies the vehicle that collected the measurement described by the row. Aerodyne has only one vehicle and so will use "vehicle-AerodyneMobileLab"

A full list of reported parameters from the Aerodyne Mobile Lab is included in the Table Below.

7.1.1 Data file formatting

Analyzed data for each instrument will be provided in compressed comma-separated value (csv) files. One file will be generated for each organization_method name per month.

The Aclima-defined naming convention will be followed, and is described in detail in Table 8.3 in the CARB SMMI Data Management Documentation:

```
  gs://[bucket]/[organization]_[method]_[measurement
date]_[revision_number]_[revision_date]
```

E.g.

```
  gs://bucket456/aerodyne_Vocus-PTR-TOF_202509_r1_20251010
```

In addition, a readme will be included at the top level of the cloud data store to document the nature of any revisions made, starting with the first version of any uploaded file ("r1"). A second QA document in .pdf format will be uploaded and will include higher-level data QA notes as described in section 6.

7.1.2 Delivery cadence and estimated file sizing

Analyzed data will be uploaded to the bucket no later than 3 months after acquisition. Archival raw data (L0 level and similar) will be delivered via physical drive hand-delivered or mailed to CARB within 3 months of the final acquisition day of the project.

Individual file sizes are expected to vary between 5 MB for (e.g. GC-EI-ToF) and 800 MB (multiple columns of 1Hz data, e.g. Vocus-PTR-ToF). The total data burden for analyzed data is estimated at 4 GB. The total data burden including raw archival data is estimated at 3 TB.

It is most efficient to perform data analysis in batches, and so a long 6.8-week measurement campaign will likely be split in 2 or 3 batches. These splits are likely to happen mid-month, and so the data revisions may reflect the addition of new data, as opposed to a change in the original data.

7.1.3 Maintenance obligation

Aerodyne will maintain a backup of all raw and analyzed data products on our company data server for a period of at least 5 years after project finish. All analyzed data will be uploaded to the Aerodyne data bucket set up by Aclima as described above.

8. References

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Appendix A. Table of Measured Pollutants by the Aerodyne Mobile Laboratory

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	rh	62201	Relative Humidity	anem-rh	1011	Sonic Anemometer	percent
Aerodyne	press	68101	Average Ambient Pressure	anem-press	1011	Sonic Anemometer	bar
Aerodyne	temp	68105	Average Ambient Temperature	anem-temp	1011	Sonic Anemometer	degC
Aerodyne	windspeed_mps	61103	Wind Speed - Resultant	aml-ws	1011	Sonic Anemometer	meters_per_second
Aerodyne	winddir_deg	61104	Wind Direction - Resultant	aml-wd	1011	Sonic Anemometer	degrees_compass
Aerodyne	wind_x_mps	100100	wind vector - resultant	aml_windx	1011	Sonic Anemometer	meters_per_second
Aerodyne	wind_y_mps	100101	wind vector - resultant	aml_windy	1011	Sonic Anemometer	meters_per_second
Aerodyne	benzene	45201	Benzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	toluene	45202	Toluene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	benzene_ethyl	45203	Ethylbenzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	xylene_o	45204	o-Xylene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	xylenes_mp	45109	m/p Xylene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	methane_bromo	43819	Bromomethane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	butadiene_13	43128	1,3-Butadiene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	PCBTF	100001	PCBTF	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	propene_13dichloro	43841	1,3-dichloropropene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	propane_n	43204	n-Propane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	MethodCode	Method Description	Parameter Units
Aerodyne	propene	100002	Propene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	butane_n	43212	n-Butane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	butane_i	43214	Isobutane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	pentane_n	43220	n-Pentane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	pentane_i	43221	Isopentane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	octane_n	43223	n-Octane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	pentane_224trimethyl	43250	2,2,4-Trimethylpentane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	MethodCode	Method Description	Parameter Units
Aerodyne	benzene_124trimethyl	45208	1,2,4-trimethylbenzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	benzene_135trimethyl	43207	1,3,5-trimethylbenzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	benzene_123trimethyl	45225	1,2,3-trimethyl benzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	MEK	43552	methyl ethyl ketone	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	isoprene	43243	isoprene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	pinene_alpha	43256	alpha.-Pinene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	acetone	43551	acetone	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	chloroform	43803	chloroform	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	benzyl_chloride	45809	benzyl chloride	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	acetate_ethyl	43209	ethyl acetate	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	dioxane_14	46201	1,4-dioxane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	vinyl_chloride	43860	vinyl chloride	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	ethylene_trichloro	43824	Trichloroethylene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	ethylene_tetrachloro	43817	Tetrachloroethylene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	ethane_11dichloro	43813	1,1-dichloroethane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	ethane_112trichloro	43820	1,1,2-trichloroethane	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	ethylene_11dichloro	43826	1,1-dichloro ethene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	hexanone_2	100003	2-hexanone	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	acrylonitrile	43704	Acrylonitrile	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	benzene_12dichloro	45805	1,2-dichlorobenzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	benzene_13dichloro	45806	1,3-dichlorobenzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	benzene_14dichloro	45807	1.4-dichlorobenzene	GC-EI-ToF	1012	Aerodyne GC-EI-ToF-MS: Collection: Preconcentration adsorbent trap, Analysis: thermal desorption gas chromatograph mass spectrometer	ppb
Aerodyne	benzene	45201	Benzene	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	toluene	45202	Toluene	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	c8aromatics	45102	Xylene(s)	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	acrolein	43505	Acrolein	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	methanethiol	100004	methanethiol	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	dms	43915	dimethyl sulfide	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	naphthalene	45850	Naphthalene	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	acetone	43551	Acetone	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	mek	43339	Butryl-aldehyde & Methyl Ethyl Ketone	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	mvk	43558	Methyl Vinyl Ketone	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Aerodyne	c5carbonyls	100005	c5carbonyls	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction	ppb

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
						Time-of-Flight Mass Spectrometer	
Aerodyne	PM_SO4	82453	Sulfate PM2.5 STP	SP-AMS_AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ug_per_m3
Aerodyne	PM_NO3	82356	Nitrate PM2.5 STP	SP-AMS_AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ug_per_m3
Aerodyne	PM_Chl	100006	chloride PM2.5 STP	SP-AMS_AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ug_per_m3
Aerodyne	PM_Org	88350	Organic Carbon Mass PM2.5 LC	SP-AMS_AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ug_per_m3
Aerodyne	PM_Amm	88330	Ammonium Ion PM2.5 STP	SP-AMS_AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ug_per_m3
Aerodyne	PM_BC	84313	Black carbon PM2.5 STP	SP-AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ug_per_m3
Aerodyne	PM_Lead_AMS	84128	Lead PM2.5 STP	SP-AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ions
Aerodyne	PM_Arsenic_AMS	84103	Arsenic PM2.5 STP	SP-AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ions
Aerodyne	PM_Aluminum_AMS	84101	Aluminum PM2.5 STP	SP-AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ions
Aerodyne	PM_Chromium_AMS	84112	Chromium PM2.5 STP	SP-AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer:	ions

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
						Vaporization followed by EI ionization	
Aerodyne	PM_Cadmium_AMS	84110	Cadmium PM2.5 STP	SP-AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ions
Aerodyne	PM_numConc	87101	Particle Number, Total Count	CPC	1015	Butanol-based condensation particle counter, TSI 3775	num_per_cm3
Aerodyne	PM_PAHs	100007	Select PM2.5 Polycyclic Aromatic Hydrocarbons	SP-AMS	1014	Aerodyne Soot-Particle Aerosol Mass Spectrometer: Vaporization followed by EI ionization	ions
Aerodyne	Potassium	88180	Potassium PM2.5 LC	cooper-xact625	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Titanium	85161	Titanium PM10 LC	cooper-xact626	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Antimony	85102	Antimony PM10 LC	cooper-xact627	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Arsenic	85103	Arsenic PM10 LC	cooper-xact628	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Barium	85107	Barium PM10 LC	cooper-xact629	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Bromine	85109	Bromine PM10 LC	cooper-xact630	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Cadmium	85110	Cadmium PM10 LC	cooper-xact631	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Calcium	85111	Calcium PM10 LC	cooper-xact632	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Chromium	85112	Chromium PM10 LC	cooper-xact633	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Cobalt	85113	Cobalt PM10 LC	cooper-xact634	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Copper	85114	Copper PM10 LC	cooper-xact635	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Iron	85126	Iron PM10 LC	cooper-xact636	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Lead	85128	Lead PM10 LC	cooper-xact637	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Manganese	85132	Manganese PM10 LC	cooper-xact638	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	Mercury	85142	Mercury PM10 LC	cooper-xact639	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Nickel	85136	Nickel PM10 LC	cooper-xact640	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Selenium	85154	Selenium PM10 LC	cooper-xact641	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Silver	85166	Silver PM10 LC	cooper-xact642	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Thallium	85173	Thallium PM10 LC	cooper-xact643	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Tin	85160	Tin PM10 LC	cooper-xact644	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Vanadium	85164	Vanadium PM10 LC	cooper-xact645	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Zinc	85167	Zinc PM10 LC	cooper-xact646	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Aluminum	100008	Aluminum PM10 LC	cooper-xact647	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Silicon	100009	Silicon PM10 LC	cooper-xact648	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Phosphorous	100010	Phosphorous PM10 LC	cooper-xact649	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Sulfur	100011	Sulfur PM10 LC	cooper-xact650	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Chlorine	100012	Chlorine PM10 LC	cooper-xact651	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Gallium	100013	Gallium PM10 LC	cooper-xact652	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Germanium	100014	Germanium PM10 LC	cooper-xact653	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Rubidium	100015	Rubidium PM 10 LC	cooper-xact654	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Strontium	100016	Strontium PM 10 LC	cooper-xact655	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Yttrium	100017	Yttrium PM 10 LC	cooper-xact656	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Zirconium	100018	Zirconium PM 10 LC	cooper-xact657	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Niobium	100019	Niobium PM 10 LC	cooper-xact658	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	Molybdenum	100020	Molybdenum PM 10 LC	cooper-xact659	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Paladium	100021	Paladium PM 10 LC	cooper-xact660	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Indium	100022	Indium PM 10 LC	cooper-xact661	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Tellurium	100023	Tellurium PM 10 LC	cooper-xact662	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Iodine	100024	Iodine PM 10 LC	cooper-xact663	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Caesium	100025	Caesium PM 10 LC	cooper-xact664	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Lanthanum	100026	Lanthanum PM 10 LC	cooper-xact665	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Cerium	100027	Cerium PM 10 LC	cooper-xact666	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Platinum	100028	Platinum PM 10 LC	cooper-xact667	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Gold	100029	Gold PM 10 LC	cooper-xact668	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	Bismuth	100030	Bismuth PM 10 LC	cooper-xact669	820	X-RAY FLUORESCENCE XRF INSTRUMENTATION	ng_per_m3
Aerodyne	co2	42102	Carbon dioxide	ndir-co2	12	Non Dispersive Infrared Photometry	ppmv ambient
Aerodyne	o3	44201	Ozone	uvabs-o3	190	UV absorption photometry/UV 2B model 202 and 205	ppbv ambient
Aerodyne	no2	42602	Nitrogen dioxide (NO2)	caps-nox	1016	Aerodyne Cavity-Attenuated Phase-Shift (CAPS) spectroscopy Nitrogen Oxides Analyzer	ppbv ambient
Aerodyne	nox	42603	Oxides of nitrogen (NOx)	caps-nox	1016	Aerodyne Cavity-Attenuated Phase-Shift (CAPS) spectroscopy Nitrogen Oxides Analyzer	ppbv ambient
Aerodyne	hcho	43502	Formaldehyde	tildas-hcho	1017	Aerodyne Tunable Infrared Direct Absorption Spectroscopy (TILDAS)	ppbv ambient

Organization	Parameter (how it will appear in data file)	Parameter Code	Parameter Description	Method (how it will appear in data file)	Method Code	Method Description	Parameter Units
Aerodyne	eto	43601	Ethylene oxide	tildas-eto	1018	Aerodyne Tunable Infrared Direct Absorption Spectroscopy (TILDAS)	ppbv ambient
Aerodyne	ch4	43201	Methane	tildas-ch4-c2h6	1019	Aerodyne Tunable Infrared Direct Absorption Spectroscopy (TILDAS)	ppbv ambient
Aerodyne	co	42101	Carbon monoxide	tildas-co-n2o	1020	Aerodyne Tunable Infrared Direct Absorption Spectroscopy (TILDAS)	ppbv ambient
Aerodyne	h2o	100031	Water	tildas-co-n2o	1020	Aerodyne Tunable Infrared Direct Absorption Spectroscopy (TILDAS)	ppbv ambient
Aerodyne	c2h6	43202	Ethane	tildas-ch4-c2h6	1019	Aerodyne Tunable Infrared Direct Absorption Spectroscopy (TILDAS)	ppbv ambient
Aerodyne	n2o	42605	Nitrous Oxide	tildas-co-n2o	1020	Aerodyne Tunable Infrared Direct Absorption Spectroscopy (TILDAS)	ppbv ambient
Aerodyne	PM2_5	88101	PM2.5 - Local Conditions	alphaseopc	1021	Alphasense OPC-N3	ug_per_m3
Aerodyne	PM1	87111	PM1 - LC	alphaseopc	1021	Alphasense OPC-N3	ug_per_m3
Aerodyne	PM10	85101	PM10 - LC	alphaseopc	1021	Alphasense OPC-N3	ug_per_m3

Community Air Monitoring Plan Appendix G.2

California Statewide Mobile Monitoring Initiative (SMMI)
UC Berkeley Quality Assurance and Data Management Plan

UC Berkeley

aclima

Prepared by UC Berkeley
In partnership with Aclima

May 16, 2025

Contents

1. Key concepts

The University of California, Berkeley (hereafter “UCB”, “Cal”, or “Berkeley”) mobile lab (hereafter “van” or “the van”) is a mobile air quality monitoring platform for measuring air pollution operated by the Apte group at UCB.

1.1 Key Personnel

Joshua Apte, Principal Investigator (PI), Associate Professor, Department of Civil and Environmental Engineering and School of Public Health, University of California, Berkeley, Berkeley, California, USA, apte@berkeley.edu.
Responsible for high level strategy and review of sampling plans, data collection, and reporting. Will be one of the two main points of contact for transfer and sharing of the data collected from all of the instruments on board the van.

Allen Goldstein, co-Investigator (co-I), Professor, Department of Environmental Science, Policy, and Management and Department of Civil and Environmental Engineering, University of California, Berkeley, California, USA, ahg@berkeley.edu.
Assists in high level strategy and review of sampling plans, data collection, and reporting as well as VOCUS data analysis.

Maria Teresa Hernandez, Research Program Manager, School of Public Health, University of California, Berkeley, Berkeley, California, USA, mt_hernandez@berkeley.edu.
Responsible for ensuring KPIs are met in a timely and accurate manner and the research project is implemented within all constraints and requirements placed by Aclima, CARB, UC Berkeley, and all other stakeholders.

Michael Giordano, Academic Researcher, Department of Civil and Environmental Engineering, University of California, Berkeley, Berkeley, California, USA, mikegiordano@berkeley.edu.
Responsible for day-to-day operations of the van including sampling, data collection, and reporting. Alongside post-docs and graduate students in the Apte Lab, responsible for all instrumentation in the van. Will co-oversee logistics of all sampling at UC Berkeley. Will be the other of the two main points of contact for transfer and sharing of the data collected with all of the instruments on board the van.

1.2 Platform Description

The Berkeley van is a 2023 Ford Transit 250 “Medium Roof” model that has been outfitted with a custom-built cargo space and electrical system for housing and powering the equipment installed in the rear of the van. The custom electrical system includes a secondary alternator, a 2160 Ah LiFePo battery system, a power distribution system, 2 120V inverters, and a breaker and outlet system for 120V AC (and 12V DC) power distributed throughout the van interior. During operation, the system draws the majority of its required power from the secondary alternator with the battery system providing the remainder. The system can also be charged using a 50A stationary shore power line.

The interior of the van is sectioned into the personnel compartment and instrumentation compartment. In the personnel compartment, the van is always operated by a driver and an instrument operator. The driver is responsible for safe driving of the van. The instrument operator’s duties include ensuring all instruments are online and reporting and to help direct the driver in route selection during operation. The instrumentation compartment comprises the remainder of the van and is unmanned when in motion for safety reasons. The instrumentation compartment, as of April 2025, consists of the electrical system as well as two (2) 27-U racks that provide mounting points for the rack-mountable instruments (see Table 2.1) and L-track mounting bars for the remainder of the instruments, including the VOCUS. The racks are mounted on steel plates which are attached to the floor via wire rope isolators to minimize vibration interference. The instrumentation compartment also contains the entry location for the sampling lines and a supplementary air conditioning system to provide climate control for the compartment. A full description of the instrumentation can be found in Section 2. A description of the data generation from the instruments follows in Sections 1.3, 3, and 4.

1.3. PML data levels

All data from the van falls into at least one of the following data levels:

Level 0 data - raw signals and engineering data
Level 1 data - raw concentrations / mixing ratios output by each instrument
Level 2a data - raw 1s calibrated geolocated data

All instruments in the van output data at Level 1, with the exception of the Vocus PTR-TOF-MS which generates raw mass spectral data. The transformation from raw mass spectra to Level 1 and 2a data is described in Section 3.1.1. Engineering data for each of the instruments is acquired for diagnostic purposes and can be provided upon request.

1.3. Data management pipeline

Key steps in the PML's data management are summarized in Table 1.1 below.

Table 1.1: An overview of the major components of PML data management.

Data management pipeline		
1	**Publish**	Every instrument that provides serial output in the van is physically connected to a computer ("VanDAQ computer") located in the van. These connections are via a serial cable with a USB-to-serial converter, direct via a USB cable, or by Ethernet, depending on the output interfaces supported by each instrument. The majority of these connections are connected to USB hubs which connect directly to a USB port on the VanDAQ computer.

		For the non-serial output instruments (e.g. sun photometer), these are connected to analog-to-digital converters which are then connected to the VanDAQ computer in the same manner as the other instruments.
2	**Ingest**	VanDAQ is a system comprised of Linux services, PostgreSQL databases, and Python scripts that accepts and coordinates data streams from all instruments, applies and corrects timestamps, coordinates instrument data with geolocations from onboard GPS receivers, stores data in a mobile database, and transmits data in near-real-time to a stationary server's master database on the UCB campus. The system is described in more detail in section 2.
3	**Transform**	Data is currently queried from the central stationary server and automatically written as long-form (one data point per row with metadata) CSV data files on a per-day basis. Future required data products such as differently formatted files or live network data feeds are easily fitted into the output scheme.
4	**Model**	See Aclima documentation.
5	**Store**	Data is stored redundantly at several junctures along the pipeline: 1) The mobile server's PostgreSQL database, "submission files" written by the van server and transmitted to the central stationary server via network on a one-minute bases, stored both 2) on the van server and 3) on the central server, 4) on the central server's PostgreSQL database, 5) in text files queried from the central database and stored on the central server, and 6) in Google Cloud archive storage automatically backed up from the central server.

2. Methods and Equipment

2.1 Instrumentation

Instrumentation for the van falls into 3 broad categories: gas-phase measurements, particle-phase measurements, and supplementary measurements. The make, model, parameters measured, limit of detection (LoD), AQS codes (where applicable), and location of each instrument is listed below in Table 1.1. LoD's are determined either through manufacturer-provided documentation or through calculation (2 times the standard deviation during a blank or zero measurement).

Table 2.1 Instrumentation Installed in the UC Berkeley Van

Make	Model	Parameter(s) Measured	AQS Code(s)	Limit of Detection (at sampling interval)	Location
Aeris	MIRA Ultra CH_4/C_2H_6	1. CH_4 2. C_2H_6 3. H_2O	1. 43201 2. 43202 3.	1. 10 ppb (1s) 2. 1 ppb (1s)	Gas-rack
Aeris	MIRA Ultra CO/N_2O	1. CO 2. N_2O 3. H_2O	1. 42101 2. 42605 3.	1. 1 ppb (1s) 2. 1 ppb (1s)	Gas-rack
Ecophysics	nCLD 855	1. NO 2. NO_2 3. NO_X	1. 42601 2. 42602 3. 42603	1. 0.4ppb NO (1s) 2. 0.4 ppb NO_2 (1s) 3. 0.4 ppb NO_X (1s)	Gas-rack
Aerodyne	CAPS NO2	NO_2	42602	<1 ppb (1s)	Gas-rack
2B Tech	211 G	O_3	44201	1 ppb (1s)	Gas-rack
Licor	LI-7200 RS CO2/H2O	1. CO_2 2. H_2O	1. 42102 2.	1. 0.3 ppm (1s) 2. 0.01 mmol/mol (1s)	Particle- rack
Palas	FIDAS	1. PM_1 2. $PM_{2.5}$ 3. PM_{10} (N/A in current setup)	1. 87111 2. 88101 3. 85101	0.001 ug/m^3 at particle sizes above 180nm (1s)	Particle- rack
Droplet Measurement Technologies	PAX (Photoacoustic Extinctiometer)	Black carbon mass	84313	< 1 Mm^{-1} Absorption and scattering of black carbon (1s)	Particle- rack
Magee	Aethelometer	Black carbon mass	84313	< 0.005 µg/m^3 (1hr avg)	Particle- rack
TSI	wCPC 3789	Total Suspended Particulates	(n/a)	50% counting efficiency at 2.2nm (1s)	Particle- rack
Aerodyne	VOCUS	1. benzene 2. toluene 3. sum of ethylbenzene and xylenes 4. acrolein 5. methane thiol 6. dimethyl sulfide 7. napthalene 8. Sum of acetone and propanone 9. methyl ethyl ketone	1. 45201 2. 45202 3. 45102 4. 43505 5. 6. 43915 7. 45850 8. 43551 9. 43339 10. 43558 11. (n/a) 12. (n/a)	1. 50 ppt 2. 10 ppt 3. 5 ppt 4. 80 ppt 5. 1500 ppt 6. 10 ppt 7. 30 ppt 8. 50 ppt 9. 30 ppt 10. 30 ppt 11. 20 ppt 12. 400 ppt	L-Track

		10. methyl vinyl ketone 11. C5 Carbonyls 12. ethanol		(all 1s)	
Airmar	WX200	1. Wind Speed 2. Wind direction 3. Ambient Temperature 4. Ambient Pressure	1) n/a 2) n/a 3) n/a 4) n/a	1) n/a 2) n/a 3) n/a 4) n/a	Roof
MetOne	Solar Radiation Sensor Model 094	Incoming solar radiation	(n/a)	5mV/kW/m^2 (1s)	Roof

2.2 Sampling Inlet Descriptions

The particle and gas inlets are installed such that all are oriented towards the front of the van at an elevation of approximately 7 feet (2.1 m) off the ground and begins just behind the front bumper of the van. This sufficiently removes the inlets from the slipstream of the vehicle itself and allows for sampling at just above breathing zone height. All sampling tubes are connected to a piece of aluminum, for rigidity, which is connected to mounting bars on the roof of the van. All sampling tubes enter the van through a single custom-manufactured bulkhead flange.

2.2.1 Particle Inlet

The particle instruments (FIDAS, wCPC, PAX, Aethelometer) all draw sample air off a single inlet constructed from primarily ⅜″ stainless steel. On the exterior of the van, on the roof, the particle line passes through a nafion dryer (PermaPure PD-50T-12MSS) which is fed a counterflow of dry air from the inside of the van. The dried sample is then passed through a singular hole in the bulkhead flange into a region where a PM$_{2.5}$ cyclone (MetOne) can be installed or removed. The particle line then passes through a region with an installed HEPA filter that can be turned on for “zeros” at any time during operation. The lines are then split using precision manufactured flow splitters (Brechtel Manufacturing Inc.) to enter into each of the particle instruments and the Aclima node. A particle loss calculator[1] was used to confirm that the 50% transmission efficiency of the system is 4 µm and the transmission of PM$_{2.5}$ is approaching 100%.

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[1] Drewnick, F., Particle Loss Calculator, Retrieved from: https://www.mpic.de/4230607/particle-loss-calculator-plc

2.2.2 Gas Inlets

The gas-phase instruments (VOCUS, all gas-rack located instruments, and LiCor) are fed through 3 different Teflon tubes that are mounted to the stabilizing aluminum bar, in the same fashion as the particle inlet, and then enter the van via individual holes in the bulkhead flange. The VOCUS and gas-rack instruments lines are ¼" Teflon while the LiCor uses a ⅜" line due to different flowrate and pressure drop requirements. The Aclima node in the van also draws off the LiCor inlet. The VOCUS line is backed by a separate pump pulling at 5 lpm to reduce the residence time in the line to be equal to that of the gas-rack line. All gas inlets have a residence time of less than 1 second.

3. Data ingestion

Data ingestion for the UCB van is performed by a custom-designed data acquisition system referred to as VanDAQ. The architecture of this Linux/Postgres/Python/Apache system is diagrammed in Figure 3.1.

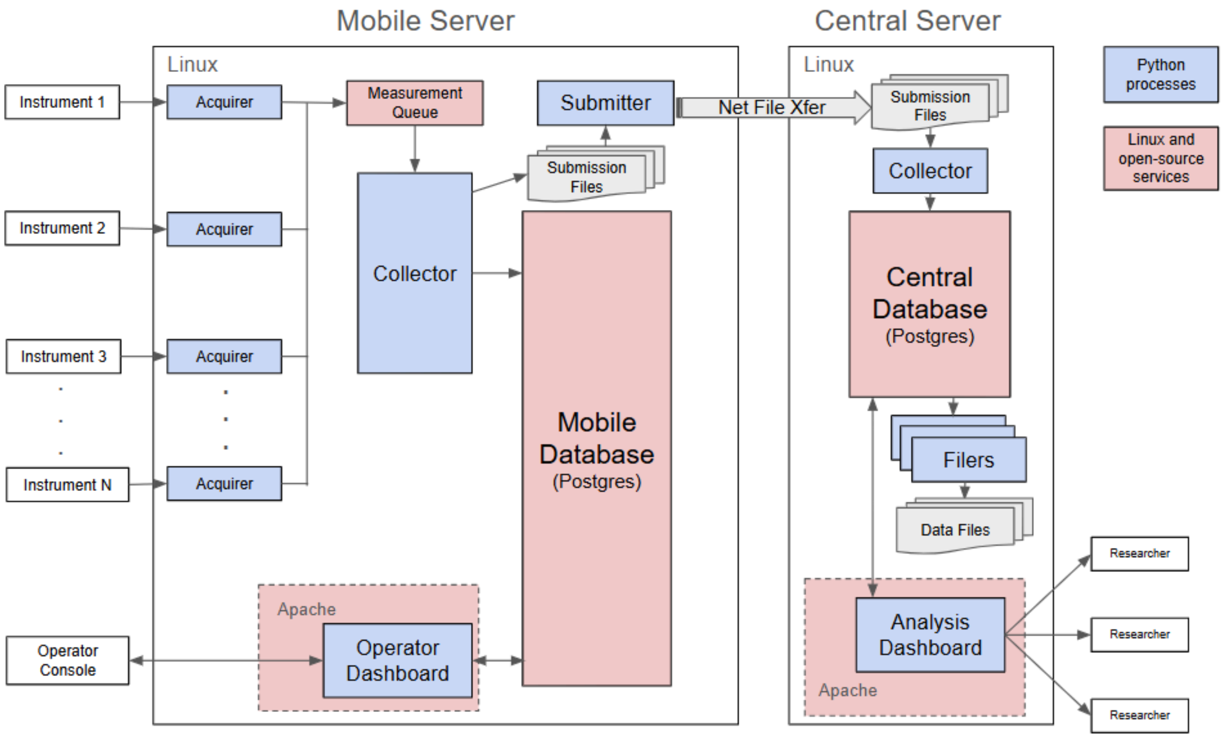

Figure 3.1: VanDAQ system architecture.

The VanDAQ system consists of a mobile Linux server in the van and a stationary central Linux server located in the Apte Lab on UCB's campus. A number of Python software processes facilitate data transfer from the instrument feeds to a Postgres database in the van. The data is then transmitted over a file-based cellular+WiFi data link to the central server which ingests mobile data into the central database. The architecture can support multiple mobile servers and, potentially, stationary data collection platforms running the same software, all reporting data to the central server.

Each instrument in the mobile platform is serviced by an **acquirer** process. The acquirer is a Python script that is configurable via a text file to acquire data based on the data link style, protocol, and format unique to each instrument. Both environmental measurement and instrument engineering values are acquired. There is only one acquirer code body that is launched into multiple processes configured to each instrument. The acquirer is the only software component in the system that "understands" the unique communication needs of the instruments, converting the data into a common-currency exchange format consisting of a Python dictionary for each individual data value and metadata describing the source, type, parameter, and unit of the data item. The unified and packaged measurement data are loaded by the various acquirer processes into a single Posix interprocess communications queue, the **measurement queue**, for further processing downstream. This feature of the VanDAQ architecture facilitates the incorporation of various diverse instruments without change to the rest of the system downstream of the acquirer. Instrument alarms and warnings are also handled by the acquirer and are packaged along with their associated data items.

The measurement queue is unloaded by the **Collector** process which 1) loads the data items into the mobile server's PostrgeSQL database and 2) packages the measurement dictionaries into one-minute *submission* data files for transmission to the central server. As the Acquirer is the only process that knows how instruments communicate, the collector is the only component that deals with the intricacies of loading the SQL database.

In the van, the server runs an operator **dashboard** website which is published through Apache and available via the van's internal WiFi network. The dashboard displays graphical time series of measurement parameters produced by all instruments, alarm states, and a real-time street map with data tracks.

The submission files are transferred via cellular or WiFi link (depending on the availability of campus WiFi) to the central server by the **Submitter** process. Submission of data files to the central server is asynchronous and can deliver data for ingestion into the central database in near-real-time (1+ minute latency) or, depending on the state of the mobile network link, will store data files and submit when possible. Another collector process on the central server ingests data from the submission files, instead of a message queue, and inserts measurements into the central database, whose schema is a duplicate of the mobile database(s).

On the central server, various **Filer** processes query the database and create text data files in various desired formats. Data processing scripts producing derived data products are included at this position of the data chain. The central server also hosts an analysis dashboard website allowing researchers to browse historical data, monitor the current state of the van, and observe mapped data collection in near-real-time. (While the analysis dashboard is currently the same as the van operator dashboard, these functions will diverge in the future.)

4. Data transformation

There are 2 data transformation steps taken in the van. The first is applying calibrations The main data transformation for instruments in the van occurs before the ingestion and storage stages but is described here.

4.1. Data transformation workflows

4.1.1. Processing Vocus PTR-TOF-MS data

4.1.1.1. High resolution mass spectral peak fitting

Half hourly, raw mass spectral data from the Vocus PTR-TOF-MS is transformed via standard, well established practices within the Tofware analysis software by an analyst in the UCB team. The following steps are taken in chronological order to return ions per second of each mass of interest:

1) File by file mass calibration using common m/z peaks present in ambient air samples
2) Baseline subtraction
3) Peak width and shape refinement
4) Mass spectral peak fitting and integration of selected mass peaks

4.1.1.2. Conversion to concentration values

Ion counts for each mass are then converted to concentration values via the use of a gas calibration standard of 13 VOCs, a zero air generator and mass flow controllers for varied dilution. Multipoint calibration curves and zeros are generated weekly to calculate sensitivities for each of the 13 VOCs. For VOCs not included in the calibration standard, sensitivities are estimated from a mass dependent transmission function and a linear relationship between sensitivity and the PTR reaction coefficient of each species, both derived from the 13 calibrated species. If the reaction coefficient is not known, then a k_{PTR} coefficient of 2.5×10^{-9} molec cm^{-3} s^{-1} is used. In addition, instrument drift due to detector and reactor conditions between calibrations is corrected for by normalisation to m/z

116.9 (CCl_4+) counts. CCl_4+ is a CFC product ion that is stable in the atmosphere as a result of the Montreal Protocol and thus can act as an internal standard. The uncertainties associated with these calibrations are reported with the Level 2a data.

5. Data modeling

See Aclima documentation.

5.1. Data modeling workflows

See Aclima documentation.

6. Data storage

Data is stored redundantly at several junctures along the data handling pipeline: including in PostgreSQL databases on the mobile [1] and central [2] servers, in “submission files” written by the van server and stored both there [3] and on the central server [4], in text files queried from the central database and stored on the central server [5], and in Google Cloud archive storage automatically backed up from the central server using rclone software [6].

Server storage, both mobile and central, is on SSDs. The mobile server is fitted with two 4TB SSDs as discrete volumes. The central server uses four 4TB SSDs in a RAID organized as two RAID1 mirrored 4TB volumes.

Vocus PTR-TOF-MS h5 files are stored on the instrument itself and then backed up to the same Google Cloud storage described above.

VanDAQ code and configurations are mastered in a repository on UCB’s Enterprise GitHub site.

7. Data review and quality assurance

After every drive, time series plots of all collected measurements, including instrument engineering parameters, and concentration maps are automatically generated for review. These plots are checked by trained operators for common signs of instrument failure, such as discontinuities, continually increasing/decreasing baselines, random noise spikes (outliers unsubstantiated by other instruments), and non-responsiveness. Additionally, each instrument is examined for overall stability relative to performance during previous deployment and non-deployment periods. Acceptance criteria and potential corrective actions are described below.

Gas-phase instruments are calibrated weekly against certified gas standards. Calibration standard documentation is available from UCB but, briefly, includes gas cylinders sourced from Airgas, a zero air generator from Teledyne, and a 2BTech ozone/NO/NO_2 calibration system (Model 714). The gas cylinders include:

Table 7.1: Calibration cylinder contents and associated instruments

#	Contents	Associated Instrument(s)	Calibration Schedule
1	VOC gas blend of 1 ppm 1,3-butadiene, 1,3,5-trimethyl benzene, 1 ppm acetaldehyde, 1 ppm acetone, 1 ppm acrylonitrile, 1 ppm ethanol, 1 ppm hexane, 1 ppm isoprene, 1 ppm limonene, 1 ppm m-xylene, 1 ppm methyl ethyl ketone, 1 ppm methyl vinyl ketone, 1 ppm toluene	Vocus PTR-TOF-MS	1x Weekly
2	5 ppm NO	CAPS NO_2 and Ecophysics NO/NO_2/NO_x	1x Weekly
3	1.9 ppm CH_4, 400 ppm CO_2, 0.1 ppm CO	Aeris CH_4/C_2H_6, Licor CO_2, Aeris CO/N_2O	1x Weekly
4	30 ppm CH_4, 1 ppm C_2H_6, 2000 ppm CO_2, 10 ppm CO	Aeris CH_4/C_2H_6, Licor CO_2, Aeris CO/N_2O	1x Weekly

Zero and slope values are generated from the multi-point calibrations for each instrument and applied to the raw concentration data via linear interpolation. If any repairs or modifications are done to instruments, calibrations are performed immediately afterwards in addition to the normal weekly schedule.

Weekly baseline readings are measured for particle phase instrumentation via the use of a Hepa filter on each instrument’s inlet. A baseline subtraction is performed for each instrument via linear interpolation.

7.1 Data Quality Metrics and Acceptance Criteria

7.1.1 Data Recovery

Data recovery is defined as the number of valid measurements collected divided by the number of total possible measurements, as a percent:

$$Data\ Recovery\ (\%) = \frac{N_{valid\ data}}{N_{possible\ data}} * 100$$

where $N_{valid\ data}$ is the number of data points obtained and $N_{possible\ data}$ is the number of theoretically possible data points. For each individual day or drive, the acceptance criteria for field measurements data recovery is 90%. If data recovery targets are not met for an individual day or drive, the drive is not marked as complete and the drive is repeated after whatever issue(s) caused data loss is addressed.

7.1.2 Precision

Precision, or the repeatability of measurements, is estimated in different ways for different instruments. For trace gas monitors (O_3, NO_2, etc.), precision checks are completed as part of the span checks described above. For the PM monitors, intra-unit precision is calculated where possible (i.e. overlapping measurements) by comparing the relative standard deviation of each instrument as per South Coast Air Quality Management District’s evaluation procedure for sensors at AQ-SPEC.

No rejection criteria is set for precision, as different measurement technologies are sensitive to different factors, but all are reported on a regular basis. Changes in precision of more than 10% on a week-to-week basis, or 25% over a month-to-month basis, will result in a full diagnostics check of the affected instrument. Manufacturer suggested maintenance will be performed, and, if necessary, instruments will be shipped back to the manufacturer for repair.

7.1.3 Accuracy

Accuracy will be determined by evaluating instrument responses to repeat analysis of gas samples containing known concentrations of the compounds of interest, as described above.

No specific metric nor rejection criteria is set for accuracy, as different measurement technologies are sensitive to different factors, but performance will be monitored as part of the regular calibration procedures. In some cases, it may be necessary to perform in-house maintenance, based on manufacturer guidance, or ship equipment to the manufacturer for repair in order to address more substantial loss of accuracy.

7.2 Data Alarms and Data Impact

In addition to post facto checks by trained personnel (described above), all instruments in the van are automatically monitored during data acquisition for potentially problematic data records during normal operation, calibrations, and idling. Each instrument has a list of conditions that may indicate faulty operation, such as internal temperatures falling outside of defined normal operating bounds or an instrument internal error flag being raised. When potential error conditions are met, the “alarm” table in the data schema (see Section 8.1) is populated with the alarm type and other relevant information.

Not all alarms immediately impact data. Some alarms exist to notify van operators that instruments are still in acceptable operating conditions but some preventative steps (e.g. turning down the air conditioning temperature) should be taken. Each alarm therefore has an associated “data_impacted” field which is “True” if a specified condition of an instrument renders the data unusable. A common example is when an instrument is entering an auto-zero mode, such as the CAPS. Instrument conditions that record “alarms” but do not necessarily impact the data are recorded in the alarm table with “data_impacted = False”. Likewise, manual review by trained personnel as described above also sets “data_impacted=True” where appropriate.

7.3. Data revisions

Submitted data values will not be altered, but potentially faulty data, identified using the methods described above, will be flagged in the “status_indicator” column in submission files transmitted to Aclima. See below for a description of how the data field is populated.

Data revisions beyond what is outlined above are not anticipated. However, any revisions will be labeled according to naming conventions described in Section 8.1.1 with an additional “_revX”, X indicating the revision number, and will be accompanied by documentation describing the revision/s.

8. Data transfer

See Aclima documentation for direct-to-CARB data transfer. UCB to Aclima data transfer will be handled automatically through FTP or similar file transfer mechanisms.

8.1. Data Schema

VanDAQ's Postgres database utilizes a star schema visualized in Figure 8.1.

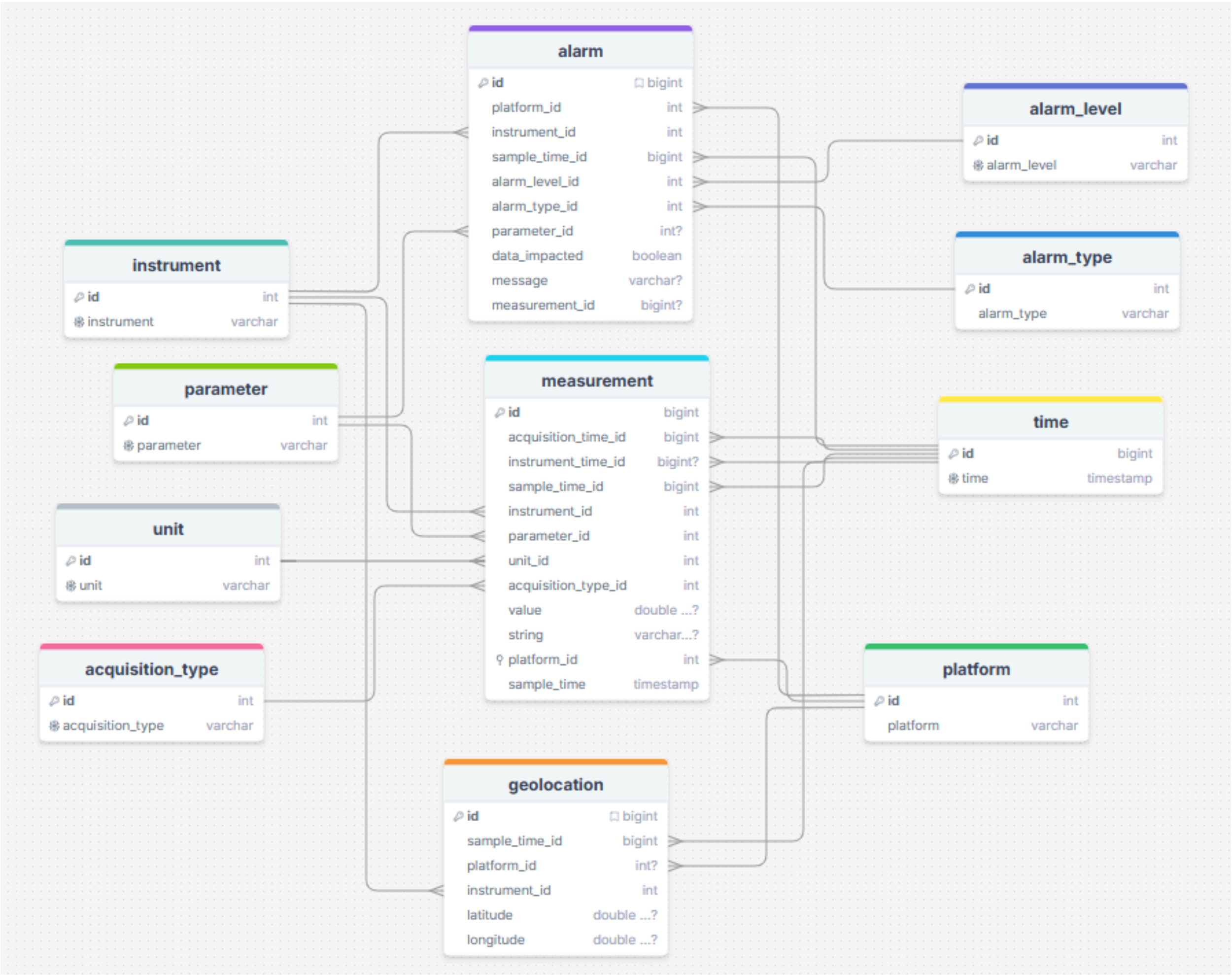

Figure 8.1: VanDAQ database schema

Files transmitted to Aclima will be csv's with the following column headings. A mapping of the above data schema to the file transmitted to Aclima is provided below:

Table 8.1: VanDAQ to Aclima Mapping table

Aclima Column Name	VanDAQ Output Equivalent Mapping
Timestamp	time/time
Modality	parameter/parameter
Model	instrument/instrument
Value	measurement/value

Unit	unit/unit
Latitude	geolocation/latitude
Longitude	geolocation/longitude
Status_indicator	0 if data_impacted = False, 1 if data_impacted = True (see Section 7.2)
qualifier_codes	alarm* (see Section 8.1.2)
Vehicle_id	No direct map, constant “UCB”

8.1.1. Data file formatting

Filename conventions follow the form “measurements_van1_yyyy-mm-dd_long.csv” where yyyy, mm, and dd are year, month, and day, respectively. All data, with the sole exception of VOCUS raw mass spectra, will be submitted as csv files. VOCUS raw spectra will be submitted as h5 files that the instrument natively outputs.

8.1.2 Qualifier Codes

The normal output schema for VanDAQ evaluates each parameter’s potential error indicators as separate alarms. For reporting purposes, this VanDAQ output is flattened and mapped such that each alarm (automatic and manual) is assigned a unique value. The linear addition of all of the alarm values is reported in “qualifier_codes” for each data record for each instrument:

$$Qualifier\ Code = \sum(Individual\ Qualifier\ Codes)$$

A full list of codes is provided elsewhere, but examples are shown below in Table 8.2:

Table 8.2: Qualifier_code example values

Instrument	Indicator	Qualifier_code Values
(all)	Operator review indicates problem	1
VOCUS	TPS temperature 20 > T > 48 °C	2
VOCUS	TPS temperature T > 50 °C	4
VOCUS	H_2O Flowrate 14.9 > F > 15.1 sccm	8
VOCUS	Ion Source Voltage 415 > V > 430	16

CAPS NO_2	Instrument currently in automatic baseline period	2
CAPS NO_2	Instrument temperature 20 > T > 40 °C	4

As the qualifier codes are all powers of 2, the linear combination of all codes at any given time is a unique value that can be decomposed to its constituent parts. If a VOCUS data record has an ion source voltage of 412V and a TPS temperature of 49, the qualifier_codes applied would be:

$$Qualifier\ Code\ =\ 16\ +\ 2\ =\ 18$$

If that same data record is flagged by an operator:

$$Qualifier\ Code\ =\ 16\ +\ 2\ +\ 1\ =\ 19$$

This method can be paired with a lookup table to identify each individual error code. Alternatively, the data can simply be filtered for records where "Status_indicator" and "qualifier_code" are both equal to 0.

8.2 Reporting

Deliverables to Aclima will include:

1) The data, as described above, and
2) QA results

The cadence of data delivery is described below. QA results will be submitted every 3 months.

8.2.1. Delivery cadence and estimated file sizing

Data delivery is performed weekly with estimated file sizes on the order of 500mb/day or 6.5gb/week. Raw h5 files will be produced at the end of the project in a physical harddrive delivered to Aclima and/or CARB. More frequent h5 file deliveries can be arranged upon request.

8.2.2. Maintenance obligation

Data is maintained indefinitely but will be archived after 1 year, at which point data will be accessible through a request to UCB.

Appendix A. Table of Measured Pollutants by the Berkeley Mobile Laboratory

Organization	Parameter	Parameter Code	Parameter Description	Method	Method Code	Method Description	Parameter Units
Berkeley	Benzene	45201	benzene	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	Toluene	45202	toluene	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	C8Aromatics	45102	sum of ethylbenzene and xylenes	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	Acrolein	43505	acrolein	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	CH4S		methane thiol	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	DMS	43915	dimethyl sulfide	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	Naphthalene	45850	Napthalene	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	C3H6O	43551	Sum of acetone and propanone	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	MEK	43339	Methyl ethyl ketone aka 2-butanone	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb

Berkeley	MVK	43558	Methyl vinyl ketone	Vocus-PTR-ToF	1013	Aerodyne Vocus Proton Transfer Reaction Time-of-Flight Mass Spectrometer	ppb
Berkeley	CO2_ppm	42102	CO2	Licor	ndir-co2	Non Dispersive Infrared Photometry	ppmv ambient
Berkeley	H2O_LC		H2OMRV	Licor	licor-h2o	Non Dispersive Infrared Photometry	ppbv ambient
Berkeley	O3	44201	O3	2BTech	uvabs-o3	UV absorption photometry/UV 2B model 202 and 205	ppbv ambient
Berkeley	NO2_CAPS	42602	NO2	CAPS-nox	caps-nox	Aerodyne Cavity-Attenuated Phase-Shift (CAPS) spectroscopy NO2 Analyzer	ppbv ambient
Berkeley	NO2	42602	NO2	EP_nox	ecophysics-no2	Ecophysics nCLD 855 Y Nitrogen Oxides Analyzer	ppbv ambient
Berkeley	NO	42601	NO	EP_nox	ecophysics-no	Ecophysics nCLD 855 Y Nitrogen Oxides Analyzer	ppbv ambient
Berkeley	NOx	42603	NOx	EP_nox	ecophysics-nox	Ecophysics nCLD 855 Y Nitrogen Oxides Analyzer	ppbv ambient
Berkeley	CH4	43201	CH4	AerisCH4	aeris-ch4c2h6	Aeris MIRA Ultra CH4	ppbv ambient
Berkeley	C2H6	43202	Ethane	AerisCH4	aeris-ch4c2h6	Aeris MIRA Ultra CH4	ppbv ambient
Berkeley	H2O_ACH4		H2OMRV	AerisCH4	**aeris-ch4c2h6**	Aeris MIRA Ultra CH4	ppbv ambient
Berkeley	CO	42101	CO	AerisCO	aeris-con2o	Aeris MIRA Ultra CO	ppbv ambient
Berkeley	N2O	42605	N2O	AerisCO	aeris-con2o	Aeris MIRA Ultra CO	ppbv ambient
Berkeley	H2O_ACO		H2OMRV	AerisCO	aeris-con2o	Aeris MIRA Ultra CO	ppbv ambient
Berkeley	PM2_5	88101	PM2.5 - Local Conditions	Palas	1021	Palas Fidas 200	ug_per_m3
Berkeley	PM1	87111	PM1 - LC	Palas	1021	Palas Fidas 200	ug_per_m3
Berkeley	PM10	85101	PM10 - LC	Palas	1021	Palas Fidas 200	ug_per_m3
Berkeley	rh	62201	Relative Humidity	anem-rh	1011	Airmar WX200	percent
Berkeley	press	68101	Average Ambient Pressure	anem-press	1011	Airmar WX200	bar
Berkeley	temp	68105	Average Ambient Temperature	anem-temp	1011	Airmar WX200	degC

Berkeley	windspeed_mps	61103	Wind Speed - Resultant	aml-ws	1011	Airmar WX200	meters_per_second
Berkeley	winddir_deg	61104	Wind Direction - Resultant	aml-wd	1011	Airmar WX200	degrees_compass

Community Air Monitoring Plan Appendix G.3

California Statewide Mobile Monitoring Initiative (SMMI) UC Riverside Team Quality Assurance and Data Management Plan

Prepared by UC Riverside, University of Houston, and Baylor University
In partnership with Aclima

May 16, 2025

Contents

1. PROJECT DESCRIPTION AND OBJECTIVES

1.1. PROCESS AND/OR ENVIRONMENTAL SYSTEM TO BE EVALUATED

Certain areas in California have been identified as being overburdened with air quality issues. With guidance from the California Air Resources Board (CARB), Aclima, Inc., and community stakeholders, the University of California-Riverside (UC-R)/University of Houston (UH)/Baylor University (BU) Partner Mobile Lab (PML) will conduct mobile sampling operations in many of the identified areas to address local concerns related to questions which can be reasonably be answered with the suite of trace gas, aerosol, and volatile organic compound instruments aboard the Mobile Air Quality Lab #3 (MAQL3), the areas it can access, and the duration of the sampling deployment.

2. ORGANIZATION AND RESPONSIBILITIES

2.1. KEY PERSONNEL

Don Collins, Principal Investigator, PI, Professor, Department of Chemical and Environmental Engineering, University of California Riverside, Riverside, California, USA, donc@ucr.edu. Responsible for some of the particulate analyzers. Will be the point of contact for transfer and sharing of the data collected with all of the instruments on board the MAQL. Will oversee logistics at the primary operations base at CE-CERT in Riverside.

James Flynn, Co-PI, Research Associate Professor, Department of Earth and Atmospheric Sciences, University of Houston, Houston, Texas, USA, jhflynn@Central.uh.edu.
Responsible for overall project management and reporting as well as providing oversight for instrument preparation and deployment. Will coordinate all team efforts as well as ensure the field measurements and truck are maintained and operated in a responsible manner.

Sascha Usenko, Co-PI, Professor, Department of Environmental Science, Baylor University, Waco, Texas, USA, Sascha_Usenko@baylor.edu.
Responsible for leading the AMS deployment in MAQL3 and providing operational support to the science team and for providing quality assurance oversight on Baylor measurements collected during this project.

Rebecca Sheesley, Co-PI, Professor, Department of Environmental Science, Baylor University, Waco, Texas, USA, Rebecca_Sheesley@baylor.edu.
Responsible for leading the aerosol optical measurement collection, analysis, and interpretation of the aerosol data and the apportionment of dust and biomass burning sources.

2.2. PROJECT SCHEDULE

The project timeline is given below. Note that this schedule does not include the items described in the Deliverables section below, as those Deliverables will be provided in addition to the performance of the tasks prescribed here.

Task description	Timeline
Work with Aclima on preliminary Community Air Monitoring Plans	September-December 2024
Project preparations	Receipt of Notice to Commence through the beginning of field deployment
Field Deployment	Eight consecutive weeks in the Fall of 2025
Final Data Preparation	April–May 2026

Data Reporting and Presentation	Data reporting will occur December 2025- April 2026. Collaborate with Aclima on final technical report due May 2026.

3. SCIENTIFIC APPROACH

3.1. SAMPLING DESIGN

UH MAQL3

The UH Mobile Air Quality Lab #3 (MAQL3) is a modified 2018 Freightliner Crew Cab straight truck with a twenty-four (24) feet box, forward observation deck, and articulating rooftop mounted 20-foot tower. Gas, aerosol, and meteorological measurements will be sampled from an inlet mounted to the end of the tower and stand ~30 feet above ground when raised. Four 15,000 BTU air conditioners will control the temperature and humidity in the lab space while electricity is provided by a 20kW onboard Tier 4 diesel generator. Gas phase and meteorological instrumentation housed inside the lab space and on the observation deck will measure ozone (O_3), nitric oxide (NO), oxides of nitrogen dioxide (NO_X), reactive nitrogen compounds (NO_Y), carbon monoxide (CO), carbon dioxide (CO_2), sulfur dioxide (SO_2), meteorological measurements, photolysis rate of nitrogen dioxide (jNO_2), formaldehyde (HCHO), aerosol composition and physical characteristics, and mixed layer heights.

A Handix Portable Optical Particle Spectrometer (POPS) will measure aerosol size distribution and number. Trace gas measurements of O_3, NO, nitrogen oxides (NO_X), NO_Y, CO, and SO_2 will also be collected from MAQL3. Meteorological and local condition measurements will include wind speed and direction, temperature, relative humidity, pressure, jNO_2, boundary layer height, GPS, sky conditions (all-sky camera), and forward, rear, left, and right cameras.

Figure 1. Photos of MAQL3. The upper right photo shows an example of instruments installed in the rear lab space and the lower right image shows an example of the operator stations in the cab.

Typically, the commercial and research-grade atmospheric instruments deployed are fast (1–2 s response), sensitive (good signal to noise) and selective (specific to a molecule). Output data is saved to a robust archive (in the event of unscheduled shutdown) and displays in real-time on a monitor for scientists to make in-project decisions.

3.2. GENERAL APPROACH AND MEASUREMENT PROCESSES

The Center for Environmental Research and Technology (CE-CERT) at the University of California Riverside (UCR) is the primary planned base location. There are sufficient 50-amp electrical connections at this facility, and it is located away from many interferences (e.g. industrial sources). This base location is strategically located to serve the air quality assessment of the area in and around southern California.

Weather permitting, the teams will plan to drive 5 days each week, with the remaining days allocated to instrument maintenance, calibration, preliminary data processing, and crew rest. While the duration of each driving day may vary based on the objective, the field teams are well versed in evaluating conditions and identifying objectives that can reasonably be accomplished. Initial routes will be planned to survey areas of known and likely emission sources as well as meteorological conditions. Some sources may be sampled at different times to determine if emissions vary throughout the day and/or between days. During overnight hours, instruments will remain on to expedite measurements the following day and to conduct additional instrument calibrations.

4. SAMPLING PROCEDURES

4.1. SITE SPECIFIC FACTORS

The MAQL3 is outfitted with instrumentation that samples the local air and characterizes it for a specific chemical or class of chemicals. This instrumentation runs pseudo continuously, with a constant intake flow that is processed to produce 1-second data. Anemometers and global positioning system devices also provide rapid time response information.

Once the campaign begins, the instrumentation suite will be operated continuously, switching between pre-arranged "shore" power and the on-board generator. Approximately 3 minutes are required to re-establish quality assured data following the power switches. A combination of weathervane signal along with engine operating flags will be used to identify periods of potential self sampling and will be flagged in the data files.

We plan to have shore power and a nominal base at one location (UCR) in the LA Basin area. We may also conduct measurements for extended time periods away from this base to the extent that budgets and other practical constraints allow. Prevailing and forecast meteorological conditions often influence the movements of the mobile laboratory. For source-related work we will determine which wind profiles work best for specific sources and plan accordingly. Prevailing wind conditions will contribute to decisions to move the mobile laboratory to facilities upwind of the sampling area as well. When sampling plumes upwind of the target area we will then conduct transects along the track of the plume as it progresses towards the target area. Other sampling strategies may be developed in conjunction with Aclima, CARB, and other relevant entities.

The campaign will be conducted during a two-month period. Scientists will begin to analyze the data while in the field and regularly interact with the Project Managers and others to get feedback regarding future planning while considering overall project objectives.

4.2. SAMPLING PROCEDURE

No discreet sample collection is planned for this project as all measurements are online methods.

5. MEASUREMENT PROCEDURES

O_3 will be measured by chemiluminescence (modified Thermo 42c) and UV absorption (2B Technology Model 205). NO will be measured by chemiluminescence (Thermo 42c-TL), NO_X by chemiluminescence with UV-LED NO_2 photolytic converter (Thermo 42c), and NO_Y by chemiluminescence with a heated molybdenum converter at the sample inlet (Thermo 42c). SO_2 will be measured by pulsed fluorescence (Thermo 43i-TLE) while CO will be measured by off-axis cavity ring-down spectrometry (Los Gatos 913-0024). CO_2 will be measured using a non-dispersive infrared absorption technique (Licor LI-7000). All sample lines use Teflon tubing and fittings, however stainless steel fittings are used in some situations as appropriate. With the exception of NO_Y, all inorganic trace gases are sampled through a 47 mm Teflon filter which is nominally changed weekly. NO_Y is sampled through a dedicated inlet with a molybdenum catalytic converter inlet heated to 300°C. A combination of internal pre-reactor, catalyst, or zero air overflow methods will be used to evaluate trace gas instrument baselines as appropriate for the specific instrument measurement methods.

Particle size distributions will be measured using a Scanning Mobility Particle Sizer (SMPS; custom, UCR), a Portable Optical Particle Spectrometer (POPS; Handix Scientific, Inc.), and an Aerodynamic Particle Sizer (APS; Model 3321, TSI, Inc.). The three sizing instruments have overlapping size ranges that collectively extend from about 0.02 μm to 10 μm. The three measurements will be processed together to create continuous size distributions spanning the full size range. Adjustments for the different measures of particle size (electrical mobility, optical, and aerodynamic) will be made when combining the distributions. Total particle number concentration will be measured with a condensation particle counter (CPC; Model MAGIC, Aerosol Dynamics, Inc.).

The three sizing instruments will be calibrated prior to and/or during the measurement period by sampling atomized polystyrene latex particles of known size, density, and refractive index. The concentration accuracy of the instruments (especially the SMPS) will be evaluated by comparing the number concentration calculated by integrating the size distributions with that measured directly by the CPC. Zero checks will be performed by connecting a filter upstream of the analyzer inlets.

A three-wavelength tricolor absorption photometer (TAP; Model 2901, Brechtel Inc., Hayward, CA) measures aerosol light absorption at wavelengths 365 (ultraviolet), 528 (green), and 652 (red) nanometers. TAP uses ten solenoid valves to cycle through eight filter spots and two reference filter spots. The light-emitting diode (LED) light source simultaneously shines through the sample and reference spots loaded with a 47-millimeter glass-fiber filter (Brechtel TAP-FIL100). The reference spot allows a measurement by difference approach in the TAP so the increase in light attenuation due to deposited particles on the sample spot is directly compared to the light attenuation of a reference spot. This allows attenuation by collected aerosol to be distinguished from attenuation by the blank filter. The TAP is set to rotate to the next filter spot when a filter spot's transmission reaches user-set value (Baylor uses 50%), and the reference channel gets altered whenever the sample spot is changed. Each of the eight sample spots is separated from the other by O-rings that clamp the filter material to prevent any inter-spot leakage. The air flow passes through the filter and into a solenoid valve controlled by the TAP Reader software.

Light scattering (σ_{sp}) will be measured using a TSI 3563 nephelometer (https://gml.noaa.gov/aero/maintenance/Neph_Ops_manual.pdf). In most integrating nephelometers, a white light source is used to illuminate the air sample, and light scattered by particles (and gases) at a particular wavelength is measured using a photomultiplier tube. In this project, a three-wavelength instrument is used. The TSI 3563 measures light scattering at three separate wavelengths simultaneously (450 Blue, 550 Green, and 700 Red). In addition, the TSI 3563 provides a separate measurement of particle back-scatter (σ_{bscat}). The instrument automatically calculates Rayleigh scattering from internally measured temperature and pressure and corrects the reported signal for those factors. Averaging time is matched to the TAPs and will be recalculated as needed.

The HR-ToF-AMS to be used in this study is described in detail in DeCarlo et al. (2006). Sample at atmospheric pressure enters the HR-ToF-AMS via an aerodynamic focusing lens. At the end of the lens, the collimated particle beam enters a vacuum chamber of known dimension. Within this chamber, particles achieve a terminal velocity that determines how quickly they will traverse the chamber. From this time, it is possible to calculate the particle size. At the end of the chamber, non-refractory material is vaporized and ionized by electron impact. Material is quantified using a time-of-flight mass spectrometer. The HR-ToF-AMS provides size-resolved chemical composition data at a resolution of approximately one minute. The HR-ToF-AMS operation by the Rice group is described in detail in Leong et al. (2017) and Wallace et al. (2018). Similar sampling procedures will be followed here, including the frequency of blanks and calibrations (as described subsequently). The main manifold will have a cyclone on the inlet to prevent larger material from entering the HR-ToF-AMS (which is a sub-micron instrument) and clogging the inlet pinhole. The HR-ToF-AMS will subsample isokinetically at a rate of approximately 150 mL per minute.

The calibration of the Aerodyne Research Inc (ARI) Aerosol Mass Spectrometer (AMS) is important for accurate quantification of particulate by chemical species. In order to minimize uncertainties in the reported mass concentrations, it is desirable that the fluctuations of the detection efficiency of the AMS are closely monitored and properly corrected throughout the whole campaign. The parameters that capture the AMS detection efficiency are IE_{NO3-}, which is the ionization efficiency of a reference compound—Nitrate (NO_3^-), and the air beam signal (AB), which is the ion rate (Hz) detected for a major air signal, e.g. N_2^+ in this study [*Jiménez et al.*, 2003]. While AB can be monitored continuously during instrument operation, the determination of IE_{NO3-} requires interruption of sampling to perform a calibration experiment (typically 1–2hrs). Given this restriction and the expectation (based on previous experience) that IE would not be highly variable, periodic IE_{NO3-} calibrations will be conducted during this study. Because the ratios of IE_{NO3-} to AB remains remarkably constant (r.s.d. < 1%) the continuous AB signal can be used to correct for the variations in the AMS detection efficiencies to a very good approximation.

Two other AMS parameters significantly influence the absolute values of its PM measurements: the collection efficiency (CE) and relative ionization efficiency (RIE). CE is introduced to correct for incomplete detection of nonrefractory particles, NR-PM, by the AMS, e.g., due to irregularly shaped particles that do not completely reach the vaporizer [*Jayne et al.*, 2000; *Tobias et al.*, 2000]. Although strictly speaking CE should be a function of particle size and shape, at present it is defined as the correction factor for the bulk mass concentrations, i.e., the fraction of the particle mass that is measured by the AMS. A CE value of 0.5 is assigned to sulfate, based on extensive observations from several laboratory and field tests for sulfate aerosols. The same CE value (i.e., 0.5) is applied to particles containing nitrate and ammonium, because they appear to be internally mixed with sulfate particles most of the time.

The CE value for total NR-PM_1 organics is estimated based on their size distributions, which often show two modes – a larger accumulation mode of ambient background particles that appears to be internally mixed with Sulfate Ion (SO_4^{2-}), NO_3^- and ammonium (NH_4^+), and a smaller ultra-fine mode that seems to be mainly emitted from combustion-related sources. A CE value of 0.5 is thus applied to the accumulation mode organics (due to the internal mixing with SO_4^{2-}) and CE for the smaller mode is assumed to be 1.0 because laboratory studies have shown close to 100 % AMS transmission for sooty combustion particles. By studying the size distributions of total organics, as well as individual organics mass fragments averaged over the whole sampling period, we have found that these two modes can be best separated at Dva = 160 nm and that the mass ratio of the smaller (Dva < 160 nm) to the larger mode (Dva > 160 nm) is roughly 2/3. The CE value of the bulk organics is therefore set at 0.7.

Relative ionization efficiency (RIE) is the ratio of the electron impact ionization efficiency of a given species to IE_{NO3^-} on a per unit mass basis. Note that IE_{NO3^-} is the IE of NO_3^- measured based on two major ions, m/z's 30 and 46, instead of all the mass fragments. RIE values of individual species representative have been determined in a range of laboratory measurements and tabulated [*Zhang et al.*, 2005].

Finally, two other key AMS parameters require calibration. The AMS volumetric sampling flow rate and the particle velocity. The sample flow rate will be determined using a Gilibrator II (wet bubble flowmeter). The particle aerodynamic size reported by the AMS is based on measured particle velocities. The size-velocity calibration is performed using an atomizer with an Ammonium nitrate (NH_4NO_3) solution followed by DMA size selection in the range 60–700 nm.

VOC Measurements

The rapid measurement of Volatile Organic Compounds (VOCs) on board the MAQL 3 will be key to assist in attribution of overall enhanced particle and gas phase signals to specific sources. Vehicular, biomass burning, and industrial VOC markers will all be rapidly quantified and displayed in real time informing decisions regarding the placement of both mobile laboratories to better determine sources. Three real-time VOC instruments will be deployed including PTR-MS (proton transfer reaction mass spectrometer), AROMA-VOC Mobile Trace Chemical Analyzer, and HCHO cavity ring down instrument. All three VOC instruments will be connected to a single heated Teflon® inlet (70 C).

Ionicon Analytik - Proton Transfer Reaction Mass Spectrometer (PTR-MS). The PTR-MS (QMS-300) was manufactured by IONICON Analytik, Austria (www.ionicon.com). The PTR-MS has widely served as a fast frequency atmospheric VOC analyzer for the past two decades (de Gouw and Warneke, 2007). The method applies ionization of atmospheric VOCs that have higher proton affinity than that of the water molecule (applies for most atmospheric VOCs, except alkanes) through the proton transfer reaction. Target VOCs are ionized by proton transfer using H_30+. Protonated VOCs are analyzed by a quadrupole mass spectrometer. The accuracy and precision of the measurement system has been confirmed to guarantee very low detection limits of most VOCs in the atmosphere (e.g. ~ few parts per trillion by volume (pptv); de Gouw and Warneke, 2007). Details regarding the PTR-MS operation, calibration and VOC data analysis has been previously documented by Shrestha et al 2022.

The PTR-MS will sample from a filtered, heated, Teflon® sampling line. In addition to operation in PTR mode, the MS will also be operated in SRI mode, using NO+ as reagent gases. The SRI module will be integrated with the PTR-MS to enable quick transition among reagent gases. Instrumental background will be assessed by periodically passing air over a heated catalyst for 40-60 minutes. The frequency of the background determination and calibration frequency will be determined in the field based on instrument performance and stability. As an in situ method, work with the PTRMS+SRI does not require taking any special sampling/handling precautions. The instrument in PTRMS mode operates with a nominal cycle time of 60 seconds, and the optimal cycle time for alternating among reagent gases will be assessed in the field. A logbook will be kept for instrument operators to log information on the instrument on an as needed basis. With the instrument in PTRMS+SRI mode, there will be cycling among the reagent gases which results in semi-continuous data for select VOCs. The baseline reagent gas cycling will be ~15 minute cycles per each of three reagent gases. The PTRMS+SRI will be calibrated for select VOCs every 1-5 days, depending upon the stability of the calibration curve. Previous field work during TRACER-AQ 2021 demonstrated good stability in the calibration curve over multiple days, allowing for a reduction in the frequency of calibration and a concurrent increase in the measurement schedule. The calibration of the PTR-MS will use a custom calibration system. This system employs custom calibration gas standards (typically sourced from Apel Riemer), which are diluted using mass flow controllers and zero air. The calibration curve will be assessed or rerun every 1–5 days and include five points, one of which is zero air. This curve allows for the determination of unknown ambient air concentrations based on measured response and for the assessment of instrumental parameters such as linearity, sensitivity or changes in sensitivity, and accuracy.

A sample conditioner will be used to reduce the water content of the sample. This will allow the operation of the PTRMS+SRI at a lower Townsend number and result in increased sensitivity and less fragmentation. The quantitative relationship between the PTR-MS response and known VOC concentrations as well as the dynamic linear range of that relationship is determined using a calibration curve (typically linear). ***Table 1.*** PTR-MS Method Detection Limit (MDL; ppb) and Uncertainty associated with the measured VOCs during the sampling campaign. Note: m/z dwell times range from 200 ms to 5 sec, with scan cycles ranging from 5 to 25 seconds. Sampling intervals range from 10 to 2 intervals per minute depending on the number of ions included in the sequence. Note: specific sequences developed for improved source characterization may be utilized to increase the sampling intervals. PTR-MS data will be included in the MAQL3 data sharing including level 1 data. Level 1 PTR-MS data includes the normalization of engineered data to the instrumentation reagent ion sensitivity.

Table 1: PTR-MS VOC analyte list (5 min average)

Species	***m/z***	***Uncertainty (%)***	***MDL***	***Ionization***
Acetonitrile	42	10.7	0.09	H_3O^+
Acetone	59	20.9	0.42	H_3O^+

Isoprene	69	10.1	0.15	H_3O^+
MEK	73	9.6	0.12	H_3O^+
Benzene	79	9.9	0.13	H_3O^+
Toluene	93	9.9	0.16	H_3O^+
ΣMonoterpene	137	11.2	0.52	H_3O^+
Styrene	105	11.4	0.10	H_3O^+
C3-benzene				H_3O^+
C4-benzene				H_3O^+
Xylene	107	11.1	0.18	H_3O^+
1,3-butadiene	107	11.1	0.18	NO^+

AROMA-VOC Mobile Trace Chemical Analyzer. AROMA-VOC was manufactured by Entanglement Technologies, Inc and is capable of detecting VOCs (i.e. organic compounds in the vapor phase) at the part-per-billion or greater range. The instrument utilizes cavity-ring down spectroscopy technique coupled with thermal desorption (TD). The instrument can be operated in two modes rapid scan (~5 sec sampling resolution) and analysis mode (~10 min sampling resolution; 2 min sampling and 8 min for analysis using the TD system with N_2 as a carrier gas). Rapid scan mode will provide four molecular-class channels (aromatic, diene, chlorinated and alkane) at 2-10 sampling cycles. Note: the alkane channel is very broad and may include other classes such as alcohols. Full analysis mode provide individually resolved VOC analysis of BTEX, 1,3-butadiene and isoprene and ethylene oxide (under specialized configurations). The AROMA-VOC analyzer is typically operated in rapid scan while conducting mobile measurements and analysis mode during stationary periods (e.g., overnight monitoring). The calibration of the AROMA-VOC Mobile Trace Chemical Analyzer will use the same custom calibration system and calibration gases as the PTR-MS. Calibrations are typically conducted every 1–5 days and include five points, one of which is zero air.

Picarro G2307 gas concentration analyzer. Ambient formaldehyde (HCHO) and methane (CH_4) measurements will be determined using real-time Picarro cavity ring-down instrument. The Picarro will be calibrated using methane every 1-5 days using the VOC calibration system. This instrument will be calibrated using methane diluted with zero air over five different concentration points including a zero point.

5.1 MEASURING AQS CODING

Table 2: AQS Codes for MAQL 3 Measurements

Parameter	Parameter Code	Recording Mode	Analysis Description	Anticipated Data Level
Benzene	45201	Continuous	PTR-MS	2a
Benzene	45201	Continuous	AROMA cavity ring down	2a
Toluene	45202	Continuous	PTR-MS	2a
Toluene	45202	Continuous	AROMA cavity ring down	2a
Isoprene	43243	Continuous	PTR-MS	2a
Isoprene	43243	Continuous	AROMA cavity ring down	2a
Xylene(s)	45102	Continuous	PTR-MS	2a
Monoterpenes	99000	Continuous	PTR-MS	2a
Formaldehyde	43502	Continuous	Picarro cavity ring down	2a
Methane	43201	Continuous	Picarro cavity ring down	2a
Aromatics	99003	Continuous	AROMA cavity ring down	1
m/z 27	99001	Continuous	HR-ToF-AMS	2a
m/z 28	99002	Continuous	HR-ToF-AMS	2a
m/z 43	99003	Continuous	HR-ToF-AMS	2a
m/z 44	99004	Continuous	HR-ToF-AMS	2a
m/z 57	99005	Continuous	HR-ToF-AMS	2a
Particle Number, Total Count	87101	Continuous	Condensation Particle Counter	2a
Light Absorption Coefficient	63102	Continuous	Tricolor Absorption Photometer	2a
Particle Light Scatter	88347	Continuous	TSI Nephelometer	2a
Particle size distribution	81101	Continuous	Portable optical particle spectrometer	1
Ozone	44201	Continuous	chemiluminescence	2a
Ozone	44201	Continuous	UV absorption	2a
Carbon Monoxide	42101	Continuous	Off-Axis Integrated Cavity Output Spectroscopy	2a

Carbon Dioxide	42101	Continuous	IR absorption	2a
Nitric Oxide	42601	Continuous	Chemiluminescence	2a
Oxides of Nitrogen	42603	Continuous	Photolytic-Chemiluminescence	2a
Reactive oxides of Nitrogen	42600	Continuous	Chemiluminescence with heated Mo converter	2a
Reactive Alkenes	99100	Continuous	Chemiluminescence	2a
Mixing Height	61301	Continuous	IR lidar	1
PM2.5 (SMPS)	99200	Continuous	Scanning Mobility Particle Sizer	1
PM10 (APS)	99201	Continuous	Aerodynamic Particle Sizer	1

6. QUALITY METRICS (QA/QC CHECKS)

6.1. GENERAL INFORMATION

Mobile Lab Measurements

A blended cylinder of CO, SO_2, NO, and propene will be used to challenge the majority of the instrumentation aboard the MAQL3. CO_2 measurements will be referenced to a nominally 500 ppmv standard and spanned with a nominal 1000 ppm standard. Additional discussion and impacts on data uncertainty will be addressed in the final reports as a function of combined instrument uncertainty. The blended gas challenges in the MAQL3 will be introduced automatically with a dilution system and valves to the inlet of the sample line upstream of the filter to best represent ambient conditions and account for and/or identify potential losses in the inlet lines and filter. A combination of internal pre-reactor, catalyst, or zero air overflow methods will be used to evaluate trace gas instrument baselines as appropriate for the specific instrument measurement methods.

The frequency of upscale gas dilution challenges will be determined based on pre-deployment testing. An internal scrubber further scrubs the zero-air supply to determine background conditions.

Measurement	**Zeros (nominal minimum frequency)**	**Span (nominal minimum frequency)**	**Multipoint (nominal minimum frequency)**
O3	With spans, multipoint, and hourly (chemiluminescent	Prior to sampling drives	Weekly or after instrument repair

	only)		
NO	With spans, multipoint, and hourly	Prior to sampling drives	Weekly or after instrument repair
NOx	With spans, multipoint, and hourly (chemiluminescent only)	Prior to sampling drives	Weekly or after instrument repair
NOy	With spans, multipoint, and hourly (chemiluminescent only)	Prior to sampling drives	Weekly or after instrument repair
CO	With spans and multipoint	Prior to sampling drives	Weekly or after instrument repair
SO2	With spans and multipoint	Prior to sampling drives	Weekly or after instrument repair
Reactive Alkenes	With spans and multipoint	Prior to sampling drives	Weekly or after instrument repair
PTRMS	Prior to sampling drives	Minimum of every three days	Weekly or after instrument repair
TAP	Prior to sampling drives and with white filter check	White filter check at filter change	
Neph	Prior to sampling drives	Every 15 days or after instrument repair	Every 15 days or after instrument repair (single point)
AROMA	Prior to sampling drives	Minimum of every three days	Weekly or after instrument repair
AMS	Prior to sampling drives	Minimum of every three days	Weekly or after instrument repair
Picarro	Prior to sampling drives	Minimum of every three days	Weekly or after instrument repair

Aerosol and VOC instruments will be monitored closely by MAQL 3 and remote operators to ensure continued satisfactory operation in the field. The calibration of the VOC instruments will be performed using a custom calibration system. This system employs custom calibration gas standards (typically sourced from Apel Riemer), which are diluted using mass flow controllers and zero air. The flows of the calibration gas and the VOC free dilution gas are controlled via mass flow controllers. Serial dilutions are performed by mixing 2–10 ml/min of the calibration gas into a zero-gas dilution flow of 250–400 ml/min. The calibration curve will be assessed or rerun every 1–3 days and include five points, one of which is zero air. This curve allows for the determination of unknown ambient air concentrations based on measured response and for the assessment of instrumental parameters such as linearity, sensitivity or changes in sensitivity, and accuracy. The calibration of the HR-ToF-AMS and CPC will be performed weekly (or as needed) and will include a HEPA filter zero. HEPA filter zeros will aid in the determination of minimum detection limits (two times the standard deviation of the mean zero value), which should be in the ng/m^3 range. With this frequency, the completeness of the data should easily exceed 85% barring unforeseen events such as pump or filament failure in the HR-ToF-AMS. The assumed acceptable accuracy and precision are 15% and 20%, respectively. The calibration for the HR-ToF-AMS will be conducted as follows:

- Atomize a solution of ammonium nitrate and size select particles using a differential mobility analyzer set to a specific voltage (the differential mobility analyzer will be calibrated pre-campaign using NIST-traceable polystyrene latex spheres);
- Measure the total number concentration of these particles using a condensation nucleus counter; calculate the mass concentration of ammonium nitrate assuming spheres;
- During AMS calibrations particle number concentrations will be measured using the CPC;
- Measure the particle size distribution using the HR-ToF-AMS (this will only be done at the start of the campaign and if the instrument needs to be repaired);
- Measure the ion response of the instrument to a known mass concentration of ammonium nitrate (from above); all other responses are derived from this value (this will be done weekly to monitor filament ionization and detection efficiency).

The nephelometer and TAP will sub-sample ambient air from the $PM_{2.5}$ inlet line along with the AMS and CPC. The nephelometer will be calibrated approximately every 15 days using CO_2 calibration gas and the TAP will be calibrated with each new filter (typically 3-7 days depending upon the loading). Zeros for the TAP and nephelometer will accompany the zeroing of the AMS and CPC.

Table 1. Procedures to Assess QA objective for AMS

Measurement Parameter	Analysis Method	Assessment Method
Organics, NO_3, SO_4, NH_4, Chl	AMS	Flow rate checked continuously by pressure and instrument air beam signal. Ion Signal to mass loading performed with classified ammonium nitrate aerosol (*nitrate equivalent loading*);

Table 2. Objectives and Acceptance Criteria for AMS

Analysis Method	**Assessment**	**Instrument/Parameter**	**Criteria Accuracy**	**Completeness**	**Precision**	**Corrective Action Given Failure to meet Criteria**
PM focused with an aerodynamic lens and ‘concentrated’ by differential pumping. PM vaporized with laser absorption. Gaseous PM constituents ionized with electron impact and classified by mass to charge ration	Airbeam signal Flow rate Particle time of flight pressure regime	AMS	Calibration of Relative ionization efficiency must match.	80%	NA	Flow rate restored by cleaning the orifice. Calibration performance of collection efficiency and relative ionization efficiency evaluated. Laser re-aligned according to the established procedure in the manual.

Table 3. Procedures to Assess QA objective for PTR-MS

Measurement Parameter	**Analysis Method**	**Assessment Method**
m/z = 19, 21, 30, and 32	PTR-MS and SRI-PTR-MS	Monitor reagent ion continuously. Daily air leak checks and impurity reagent ion production rates. Monitor sensitivity and linearity using select VOC m/z during calibration.

Table 4. Objectives and Acceptance Criteria

Analysis Method	Assessment	Parameter	Criteria Accuracy	Completeness	Precision	Corrective Action Given Failure to meet Criteria
Reagent ion stability and magnitude monitored with m/z = 19 and 21. Leak check monitored using m/z = 32 (O2+) Monitor reagent ion impurity using m/z 30 (NO+)	Reagent ion source voltage Ion molecule region pressure Flow rate to instrument	PTR-MS and SRI-PTR-MS	Response Factors should be within 15-20% of the running instrument performance or less than 5% for impurities	85%	Typically, 1-10 pptv at 1Hz, depending upon compound	Flow, reagent ion and pressure problem are corrected using procedure described in the PTR-MS manual

6.1.1. Detection Limit

Detection limits will be expressed in units of concentration and reflect the smallest concentration of a compound that can be measured with a defined degree of certainty. The analytical instrument detection limit (IDL) for other parameters will be established with the application of available standards according to 40 CFR Part 136, Part B, where applicable.

6.1.2. Blanks / Zeros

The system contribution to the measurement results is determined by analysis of a blank or zero air (filtered air) level as part of each calibration and span check. As part of the calibration, the zero level is used along with the upscale concentrations to establish the calibration curve. As part of the span check, the zero level is used as a quality control check for monitoring zero drift. If a method is found to have a system contribution for a target pollutant at a concentration greater than three times the detection limit or greater than 10 percent of the median measured concentration for the pollutant (whichever is larger), efforts must be taken to remove the contribution. Any system contribution for a target pollutant (or for another constituent that interferes with analysis for a target pollutant) that is above the detection limit must be thoroughly characterized such that the extent of influence on the target pollutant measurement certainty is well understood. This may require an elevated frequency of blank analyses for an adequate period to characterize the contribution. A data flag will be used when concentrations in the blank sample measurements indicate a contribution to the sample measurement result that is determined to be significant relative to the quality objectives specified for the measurement.

6.2. QUALITY ASSURANCE OBJECTIVES

The following sections describe the quality assurance objectives for this project. The findings of these activities will be included in the final reports.

6.2.1. Precision

Precision is a measure of the repeatability of the results. Estimates of precision are assessed in different ways for different measurement technologies.

Precision for measurements from continuous monitors will be estimated by analysis of a test atmosphere containing the target compounds being monitored. Precision for trace gases is estimated from precision checks that are done as part of routine span checks of the monitors. This precision check consists of introducing a known concentration of the pollutant into the monitor in the concentration range required by 40 *CFR* Part 58. The resulting measured concentration is then compared to the known concentration.

6.2.2. Accuracy

Accuracy is the closeness of a measurement to a reference value and reflects elements of both bias and precision. Accuracy will be determined by evaluating measurement system responses for replicate analysis of samples containing the compounds of interest at concentrations representative of the ambient atmospheres typically being monitored during the study as outlined in 40 *CFR* 58. Note that technical system audits are not required for a Category III QAPP.

6.2.3. Completeness

Data completeness is calculated on the basis of the number of valid samples collected out of the total possible number of measurements. Data completeness is calculated as follows:

$$\%\ Completeness = \frac{Number\ of\ valid\ measurements \times 100}{Total\ possible\ number\ of\ measurements}$$

Completeness, which measures the percentage of measurements to the number of measurements. In order to meet the objectives of the project's research plan, the acceptance criteria for field measurements and laboratory completeness is 85%, excluding QA/QC periods such as zeros/baseline checks and upscale challenges. In the event that the data completeness metrics are not achieved, a discussion of the causes and expected impacts to data interpretation and analysis will be included in the final report.

6.3. DATA AUDITING

Technical Systems Audits are not required for this project. Audits of data quality (minimum 10%) will be performed by the data processing team and designated QA representatives of each organization using visual inspection of the data, comparison of the data to the QA/QC criteria described in this document, and comparison with other measurements, as applicable. Data that passes these examinations will be deemed acceptable. Should data not pass examination on one or more of the checks, the data will be further examined by the researchers and as appropriate may be flagged as invalid, valid, or valid but having failed a check. Once the Audit of Data Quality are completed, a report of the findings will be included in the final report.

6.4. INSTRUMENT SPECIFICS

University of Houston

Mass flow controller signals will be recorded in DAQFactory software as well as valve states and the associated data flags to indicate non-ambient data during calibrations and instrument challenges. These signals will be used to calculate mixing ratios of test atmospheres for instrument sensitivity calculations.

A blended cylinder of CO, SO_2, NO, and propene will be used to challenge the majority of the instrumentation aboard the MAQL3. Additional discussion and impacts on data uncertainty will be addressed in the final reports as a function of combined instrument uncertainty. The blended gas challenges in the MAQL3 will be introduced automatically with a dilution system and valves to the inlet of the sample line upstream of the filter to best represent ambient conditions and account for and/or identify potential losses in the inlet lines and filter. A combination of internal pre-reactor, catalyst, or zero air overflow methods will be used to evaluate trace gas instrument baselines as appropriate for the specific instrument measurement methods.

The frequency of upscale gas dilution challenges will be determined based on pre-deployment testing. An internal scrubber further scrubs the zero air supply to determine background conditions.

Baylor University

All instrument parameters and data are recorded using the specific instrumental software. Post-processing of aerosol composition will be performed using Igor Pro along with Sequential Igor data Retrieval (SQUIRREL) and Pika (Peaking fitting) modules. Post-processing of the PTR-MS, TAP, NEPH, and CPC data will be performed using MATLAB. Aerosol and VOC zeros will be performed every 1-3 days using HEPA filters and zero air, respectively. System zeros will be included in the daily logs. Mass flow controllers and other parameters (inlet flowrates) will be recorded using DAQFactory or by operators in the daily logs. Daily logs and data flags will be used to identify suspect or erroneous data based on instrument outputs or periods associated with periods of MAQL 3 non-measurement activities (e.g., refueling and power transfers).

University of California Riverside

All instrument parameters from the SMPS and APS are recorded and used for post-processing of the measured size distributions. Distributions viewed in real-time are approximate solutions to the measured concentration arrays, with more accurate analysis of the data completed following each measurement day. Instrument zeros will be performed weekly by connecting filters upstream of the analyzers. Data flags will identify suspect data based on instrument parameters and extensive experience working with the instruments and the distributions they produce.

7. DATA MANAGEMENT PLAN

7.1. KEY CONCEPTS

The UC-Riverside/Baylor University/University of Houston (UCR/BU/UH) partner mobile laboratory utilizes several internal data systems for individual or groups of instruments. These data typically require different levels of processing before useful values can be produced for end users. For instance, an ambient temperature or GPS position requires minimal processing while data from mass spectrometers requires considerable time and effort to process.

7.1.1 Data Levels

Raw data – Data recorded in the instrument data system in a native format.

Level 0 data – Data that has been converted to engineering units (i.e. parts per million (ppm), parts per billion (ppb), percent) and may have been screened to exclude non-ambient data such as calibrations, baseline checks, self-sampling of mobile lab engine or generator exhaust. This data is suitable for "quick-look" type plots for sharing with other researchers within the UCR/BU/UH PML but not with personnel outside this group without PML permissions.

Level 1 data – Data that has undergone corrections for final calibration results, baseline adjustments, and a detailed inspection to remove non-ambient data and outliers. This is considered final data and suitable for sharing publicly and use in publications.

7.1.2 Data Management Pipeline

Key steps in the PML's data management are summarized in below.

Table x.x: An overview of the major components of PML data management.

Data management pipeline		
1	**Publish**	Raw data is recorded on local computer systems and inside the instruments. Data is transferred to external and online backup storage.
2	**Ingest**	Data is loaded onto the computer of an individual researcher from either an external or online backup location. The data is then loaded into a variety of software packages such as Igor Pro, MatLab, Excel, or other instrument specific applications.

3	**Transform**	Data is processed on local computers by a researcher using a variety of manual and scripted commands using a variety of software packages such as Igor Pro, MatLab, Excel, or other instrument specific applications.
4	**Model**	Derived data or "Value Added Products" are calculated using a variety of manual and scripted commands using a variety of software packages such as Igor Pro, MatLab, Excel, or other instrument specific applications. We will work in collaboration with Aclima to define a consistent approach for data modeling based on the data collected.
5	**Store**	Data is initially collected and stored on the instrument or local data acquisition systems. This data is backed up manually after each driving mission onto two external drives. A copy of the data is also uploaded to university network storage systems, such as the one owned and operated by the Flynn group at UH. This particular system is backed up nightly to a dedicated remote system in Austin, Texas. This results in at least four copies of the raw data. Each research group and university maintains their own standards for backing up work products throughout the process, including final Level 1 data, to external and/or network storage drives through a combination of manual and automatic backups.

7.2. DATA INGESTION

Data ingestion describes the process by which the unaltered lowest level data from the instruments is delivered to the PML data storage and processing backend.

7.2.1 Publish

Raw data is backed up onto duplicate external drives at the end of each driving mission. This is done either manually or through the execution of a batch file for those computers and instruments which are able to have their hard drives networked locally. These drives are then automatically uploaded to offsite storage at the universities, such as the UH storage system, when a drive is connected to a computer which is not connected to a cellular data connection, such as at the hotel where the field team is staying. In some locations, it may be possible to have a local storage device within the PML also back up the data over a 5G cellular connection, however bandwidth and data usage may not allow for this and is yet to be determined. Once uploaded to the university storage systems data will be downloaded to the computers of individual researchers for processing after collection.

7.2.2 Ingest

Raw data is loaded onto the computer of an individual researcher from either an external or online backup location. The raw data is then loaded into a variety of software packages such as Igor Pro, MatLab, Excel, or other instrument specific applications.

7.3 DATA TRANSFORMATION

Data transformation describes how data from instruments, now ingested and stored, is further transformed.

Two key levels of data are defined by the UCR/BU/UH PML team, Level 0 and Level 1.

Level 0 data – Data that has been converted to engineering units (i.e. parts per million (ppm), parts per billion (ppb), percent) and may have been screened to exclude non-ambient data such as calibrations, baseline checks, self-sampling of mobile lab engine or generator exhaust. This data is suitable for “quick-look” type plots for sharing with other researchers within the UCR/BU/UH PML but not with personnel outside this group without PML permissions.

Level 1 data – Data that has undergone corrections for final calibration results, baseline adjustments, and a detailed inspection to remove non-ambient data and outliers. This is considered final data and suitable for sharing publicly and use in publications.

7.3.1 Processing – Online measurements

Many of the online instruments such as O_3, CO, NO, NO_x, NO_y, CO_2, SO_2, and some aerosol and meteorological measurements require similar processing steps. The first step in data processing is to correct for baseline adjustments. This is done through the use of catalytic, pre-reactor, filter, or other forms of baseline checks. The data is then shifted according to the values of these periodic checks.

Once the data has been baseline corrected it is ready for the application of sensitivity based factors. These factors are developed through the calibration process which involves either supplying the instrument with a known quantity of the analyte or through comparison to a known standard.

The final step is the removal of non-ambient data through a series of scripted and manual steps to remove periods of calibration, baseline checks, self-sampling of PML exhaust, and other unrepresentative data.

7.3.2 Processing Mass Spectral Data

In unit mass resolution mode, AMS data processing begins with the collection of raw ion signals measured at integer mass-to-charge ratios (m/z). These raw spectra are imported into IGOR Pro and processed using the SQUIRREL analysis package. The initial steps involve time alignment and averaging of spectra to improve signal quality, followed by the application of calibration factors (e.g., ionization efficiency and collection efficiency) to convert ion counts into mass concentrations ($\mu g/m^3$). Within IGOR Pro, SQUIRREL uses predefined fragmentation tables and fitting routines to apportion ion signals to specific chemical species (e.g., SO_4^{2-}, NO_3^-, NH_4^+, organics; unit mass resolution). It also corrects for background signals. The output includes time-resolved mass concentrations, chemical composition summaries, and diagnostic plots (instrumental parameters), enabling further analysis and interpretation including high resolution data analysis using PIKA (also via IGOR Pro).

For a PTR-MS quadrupole instrument, the data process starts with the instrument measuring how many ions appear at different m/z ratios. These raw ion signals are first viewed and processed using PTR-MS Viewer, Ionicon’s software. Correction for drift and changes in background is performed by normalizing to specific hydronium ion (H_3O^+) and or subtract background instrumental signals using zero air gas. Once this initial processing has been performed, the data can be exported into MATLAB for more advanced data analysis and interpretation.

Raw mass spectral data will be available upon request for TOF instruments. The PTRMS will be run in select ion mode and will not have a complete mass scan available.

7.4 DATA MODELING

See Aclima’s Data Management Plan (Appendix D and E) for details on the data modeling approach for SMMI. The UCR/BU/UH PML team will work in collaboration with Aclima and the other Partner Mobile Lab teams to follow a consistent approach for analysis and presentation of the data. The general approach for data analysis and visualization is described in Aclima’s Data Management Plan (Appendix F).

7.5 DATA STORAGE

Raw data is stored on local data acquisition systems or internal instrument storage, typically as delimited ASCII text files. These data are backed up after each driving mission to external drives, typically at least two. A batch file (RoboCopy) is executed from a central display computer within the PML to transfer data from most systems to the external drives. Some instrument systems may not be compatible with the local network file sharing or batch file permissions and are backed up manually to the external drives. Time and resource permitting, a local network storage system will be installed in the PML and backup available files in near real time using either the network storage system's proprietary software, rsync, or similar software.

Data from the external drives will be backed up to university network storage systems overnight after each drive mission. Data folders will be shared with the UCR/BU/UH PML teams internally through a secure connection for download and preliminary inspection and processing.

In the case of the UH network storage system it is also backed up to a parallel system housed in Austin, TX at St. Edward's University. Through these backup processes, the data is preserved 1) on the original data system, 2) on a pair of external drives, 3) on university network storage, and 4) on off-campus cold storage, typically resulting in five parallel copies.

7.6 DATA REVIEW AND QUALITY ASSURANCE

Prior sections of this document detail the quality assurance approach in more detail. The primary tool for data review is through visual inspection by trained personnel and includes the response to calibrations. Additional screening tools such as calculating ratios of NOx:NOy, inspecting O3 response to NO plumes, and other physical and chemically representative evaluations will occur.

7.6.1 Data revisions

In the event that a data revision is required after final Level 1 data has been delivered the updated files will be named with a revision date in the file name and a metadata file describing the revision will accompany the data. The file and/or download link will be shared with the Aclima project manager so that they can notify downstream users.

7.7 DATA TRANSFER

Level 1 data will be compiled into data files following Aclima's defined schema (see Appendix X.x) and delivered to the same GCS bucket that is shared with CARB. Data delivery will occur monthly with a 3 month lag from the time of data collection.

Raw data (Level 0) can be shared with CARB as requested and will be delivered directly to CARB. Data file formats will typically identify the project name, instrument platform, species or grouping of measurements (i.e. trace gases, meteorology & GPS, VOCs, etc.), and the revision date in the file name. A header within the data files will identify the measured parameter, measurement units, and averaging times. Most of the data will be stored in delimited ASCII text formats however some data such as aerosol back scatter and backscatter gradient plots will be stored as graphical images. Final data file sizes are expected to be in the order of 10's to 100's of megabytes per day, depending on the parameter(s). Data will be maintained on the university archives for a minimum of three years after the conclusion of the project.

8. REPORTING

8.1. DELIVERABLES

Deliverables for this project will include a description of the specific reports to be submitted and their due dates are outlined below.

Preliminary Data: Preliminary data will be delivered to Aclima on a schedule which may be Daily, Weekly, Bi-weekly, or Monthly and will be determined through discussions amongst the field teams and Aclima and based on project needs, data processing requirements, and workloads.

Preliminary Data Due Date: No later than the end February 2026

Final Data: Final data suitable for analysis and publishing will be delivered to Aclima and CARB at least monthly with no more than a 3 month lag.

Final Data Due Date: Before contract end.

Interpretable Derived Products: The MAQL3 team will collaborate with Aclima and other mobile lab partners to define and create data products suitable for visualization and communication to public stakeholders.

Final Data Due Date: April 30, 2026

8.2. FINAL PRODUCT

The UCR/UH/BU SMMI PML team will collaborate with Aclima to deliver the Final Technical Report which will provide a comprehensive overview of activities undertaken during the UCR/UH/BU SMMI PML project. The Final Report will highlight major activities and key findings, including the Audit of Data Quality, provide preliminary analysis, describe encountered problems and associated corrective actions, and detail relevant statistics, including data completeness, accuracy, and precision.

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